Provisional Maturity Science Review For NOAA-20 OMPS Ozone Profile EDR – V8Pro

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JPSS NOAA NASA

Disclaimer

"The contents of this presentation are mine personally and do not necessarily reflect any position of the US Government or the National Oceanic and Atmospheric Administration.“

JPSS Data Products Maturity

1. Beta

- Product is minimally validated, and may still contain significant identified and unidentified errors.
- Information/data from validation efforts can be used to make initial qualitative or very limited quantitative assessments regarding product fitness-for-purpose.
- Documentation of product performance and identified product performance anomalies, including recommended remediation strategies, exists.

2. Provisional

- Product performance has been demonstrated through analysis of a large, but still limited (i.e., not necessarily globally or seasonally representative) number of independent measurements obtained from selected locations, time periods, or field campaign efforts.
- Product analyses are sufficient for qualitative, and limited quantitative, determination of product fitness-for-purpose.
- Documentation of product performance, testing involving product fixes, identified product performance anomalies, including recommended remediation strategies, exists.
- Product is recommended for potential operational use (user decision) and in scientific publications after consulting product status documents.

3. Validated

- Product performance has been demonstrated over a large and wide range of representative conditions (i.e., global, seasonal).
- Comprehensive documentation of product performance exists that includes all known product anomalies and their recommended remediation strategies for a full range of retrieval conditions and severity level.
- Product analyses are sufficient for full qualitative and quantitative determination of product fitness-for-purpose.
- Product is ready for operational use based on documented validation findings and user feedback.
- Product validation, quality assurance, and algorithm stewardship continue through the lifetime of the instrument.

Provisional Maturity Review - Entry Criteria

- Product Requirements
- Provisional Maturity Performance Validation
  - On-orbit instrument performance assessment
    - Identify all of the instrument and product characteristics you have verified/validated as individual bullets
    - Identify pre-launch concerns/waivers, mitigation and evaluation attempts with on-orbit data
- Users/EDRs feedback
- Risks, Actions, Mitigations
  - Potential issues, concerns
- Path forward to Validated Maturity
- Summary

Provisional Maturity Review - Exit Criteria

- Provisional Maturity Performance is well characterized and meets/exceeds the requirements:
  - On-orbit instrument performance assessment
    - Provide summary for each identified instrument and product characteristic you have validated/verified as part of the entry criteria
    - Provide summary of pre-launch concerns/waivers mitigations/evaluation and address whether any of them are still a concern that raises any risk.
- Updated Provisional Maturity Slide Package addressing review committee's comments for:
  - Cal/Val Plan and Schedules
  - Product Requirements
  - Provisional Maturity Performance
  - Risks, Actions, Mitigations
  - Path forward to Validated Maturity

Outline

- Algorithm Cal/Val Team Members
- Product Overview/Requirements
- Evaluation of algorithm performance to specification requirements
    - Quality flag analysis/validation
    - Algorithm improvements
    - Attempted soft calibration results
    - Algorithm version, processing environment
    - Required algorithm inputs
- User Feedback
- Downstream Product Feedback
- Risks, Actions, and Mitigations
- Documentation (Science Maturity Check List)
- Conclusion
- Path Forward

Ozone Cal/Val/Alg Team Membership

	Name	Organization	Task
Lead	Lawrence Flynn	NOAA/NESDIS/STAR	Ozone EDR Team
Sub-Lead	Irina Petropavlovskikh	NOAA/ESRL/CIRES	Ground-based Validation
Sub-Lead	Craig Long	NOAA/NWS/NCEP	Product Application
Sub-Lead	Trevor Beck	NOAA/NESDIS/STAR	Trace Gas Algorithm Development
Member	Jianguo Niu	STAR/IMSG/SRG	Algorithm development, trouble shooting, Limb Profiler science
Member	Eric Beach	STAR/IMSG	Validation, ICVS/Monitoring, Data management
Member	Zhihua Zhang	STAR/IMSG	V8 Algorithms implementation and modification
JAM	Laura Dunlap	JPSS/Aerospace	Coordination
Adjunct	Bigyani Das	STAR/AIT	Deliveries
PAL	Vaishali Kapoor	OSDPD	Atmospheric Chemistry Product Area Lead

OMPS NP EDR Performance Characteristics

Table 4.2.4 - Ozone Nadir Profile (OMPS-NP)		
Attribute	**Threshold**	**Objective**
Ozone NP Applicable Conditions: 1. daytime only (3)		
a. Horizontal Cell Size	250 X 50 km^2 (1)	50 x 50 km^2
b. Vertical Cell Size	3 km reporting	
1. Below 30 hPa (~ < 25 km)	10 -20 km	3 km (0 -Th)
2. 30 -1 hPa (~ 25 -50 km)	7 -10 km	1 km (TH -25 km)
3. Above 1 hPa (~ > 50 km)	10 -20 km	3 km (25 -60 km)
c. Mapping Uncertainty, 1 Sigma	< 25 km	5 km
d. Measurement Range		
Nadir Profile, 0 - 60 km	0.1-15 ppmv	0.01 -3 ppmv (0-TH) 0.1-15 ppmv (TH-60 km)
e. Measurement Precision (2)		
1. Below 30 hPa (~ < 25 km)	Greater of 20 % or 0.1 ppmv	10% (0 -TH)
2. At 30 hPa (~ 25 km)	Greater of 10 % or 0.1 ppmv	3%
3. 30 -1 hPa (~ 25 -50 km)	5% -10%	1%
4. Above 1 hPa (~ > 50 km)	Greater of 10% or 0.1 ppmv	3%
f. Measurement Accuracy (2)		
1. Below 30 hPa (~ < 25 km)	Greater of 10 % or 0.1 ppmv	10% (0 -15 km)
2. 30 -1 hPa (~ 25 -50 km)	5% -10%	5% (15 -60 km)
3. At 1 hPa (~ 50 km)	Greater of 10 % or 0.1 ppmv	5% (15 -60 km)
4. Above 1 hPa (~ > 50 km)	Greater of 10 % or 0.1 ppmv	5% (15 -60 km)
g. Refresh	At least 60% coverage of the globe every 7 days (monthly average) (2,3)	24 hrs. (2,3)
Notes: 1. The SBUV/2 has a 180 km X 180 km cross-track by along -track FOV. It makes its 12 measurements over 24 Samples (160 km of along-track motion). The OMPS Nadir Profiler is designed to be operated in a mode that is able to subsample the required HCS. 2. The OMPS Nadir Profiler performance is expected to degrade in the area of the South Atlantic Anomaly (SAA) due to the impact of periodic charged particle effects in this region. 3. All OMPS measurements require sunlight, so there is no coverage in polar night areas.		

Product Overview/Requirements

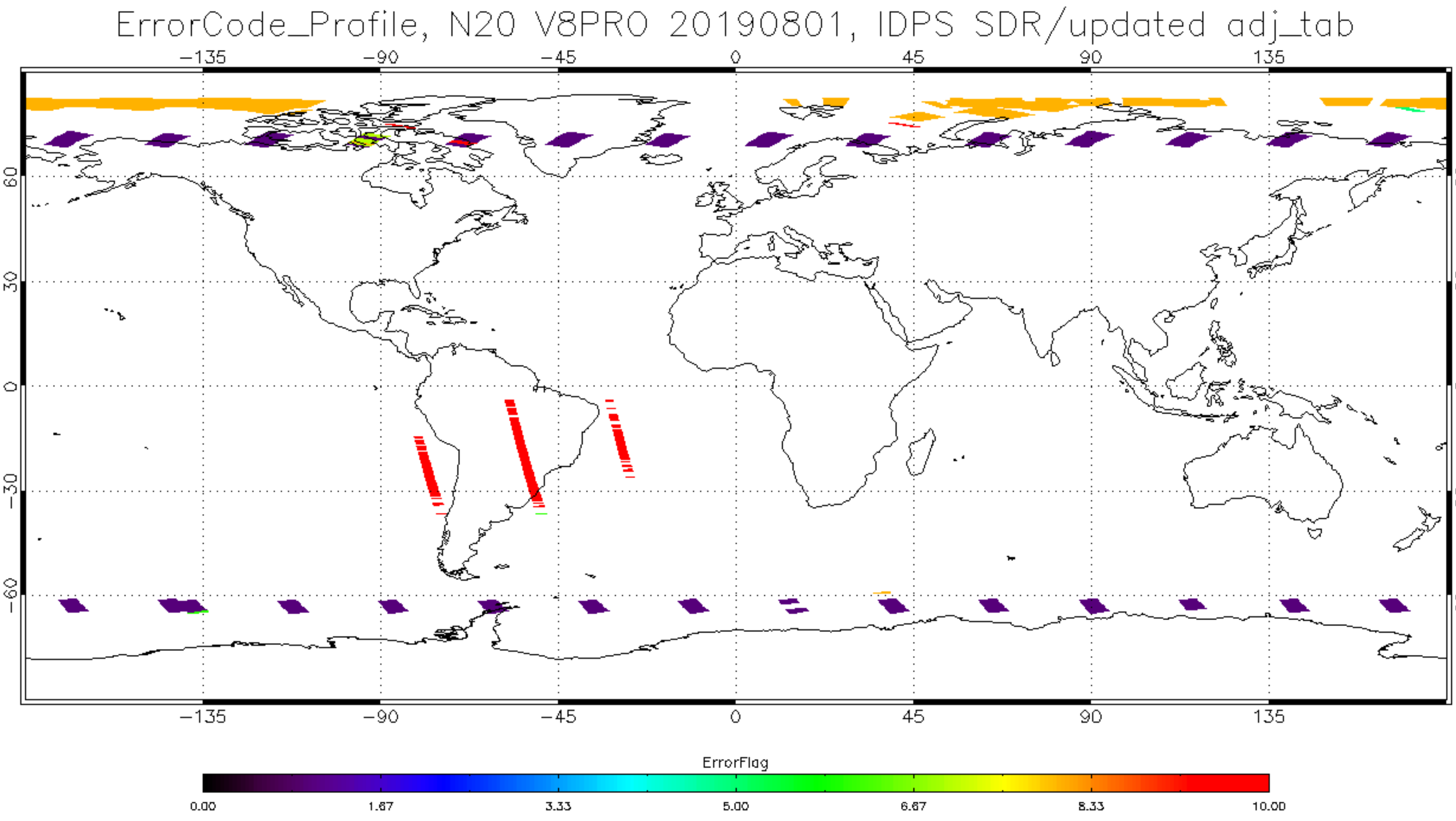
- Product performance requirements from JPSS L1RD supplement (threshold) versus observed/validated/JERD Vol. II

Attribute	Threshold	Observed/validated
Geographic coverage	60% Global Earth 7 days	SZA < 86°, orbital track
Vertical Coverage	0-60 km	0-60 km
Vertical Cell Size	3-km reporting, 7-20 km	21 layers, averaging kernel
Horizontal Cell Size	250x250 km^2	250x50 km^2
Mapping Uncertainty	25 km	5 km
Measurement Range	0.1-15 ppmv	0.1-15 ppmv
Measurement Accuracy		
h < 25 km	10%	<5% versus S-NPP in the tropics
25 km < h < 50 km	5-10%	<5% versus S-NPP in the tropics
h > 50 km	10%	<5% versus S-NPP in the tropics
Measurement Precision		
h < 25 km	20%	Measurement noise and initial and final residuals have been evaluated. The values are consistent with the expected performance and the SDR improvements.
25 km < h < 50 km	5-10%	
h > 50 km	10%	

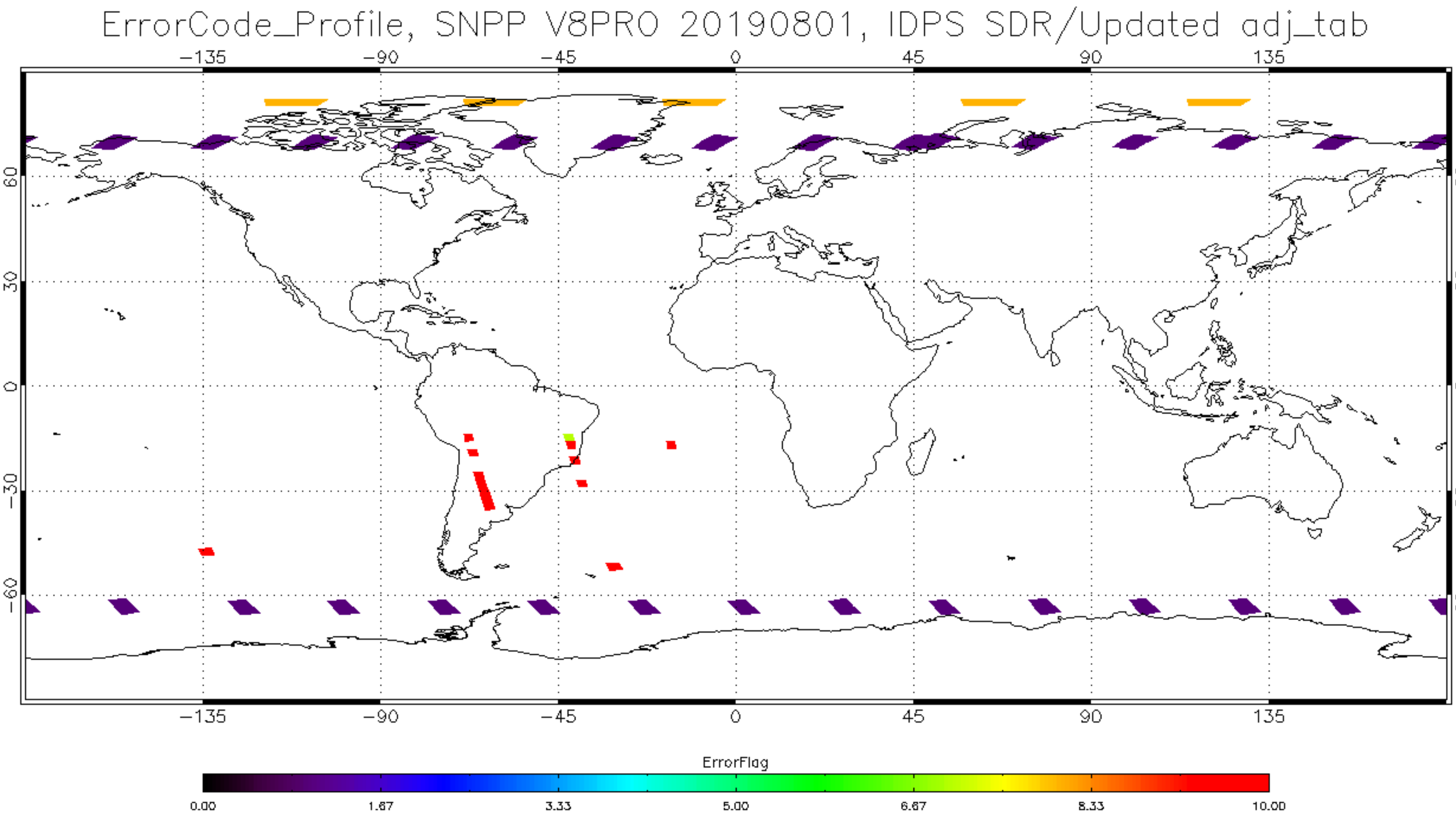
V8Pro Profile Error Code and Descriptions

<table>
<tr><th>Profile Error Code</th><th>Description</th></tr>
<tr><td>0.0</td><td>Good retrieval</td></tr>
<tr><td>1.0</td><td>SZA > 84 degrees</td></tr>
<tr><td>2.0</td><td>|Step3O3 – Profile Total| > 25 DU</td></tr>
<tr><td>3.0</td><td>Average |Final Residual| for retrieval channels > threshold</td></tr>
<tr><td>4.0</td><td>|Final residue| greater than 3 times instrument error</td></tr>
<tr><td>5.0</td><td>|Retrieved - a priori| greater than 3 times a priori error</td></tr>
<tr><td>6.0</td><td>Non-convergent solution</td></tr>
<tr><td>7.0</td><td>Stray light anomaly</td></tr>
<tr><td>8.0</td><td>Initial residue greater than 18.0 N-value units or upper level profile anomaly</td></tr>
<tr><td>9.0</td><td>Total ozone algorithm failure</td></tr>
<tr><td>+10.0</td><td>10 is added - to the flag values to designate descending portions of the orbit. The unit’s value is unchanged.</td></tr>
</table>

Profile Ozone Error Flags N20

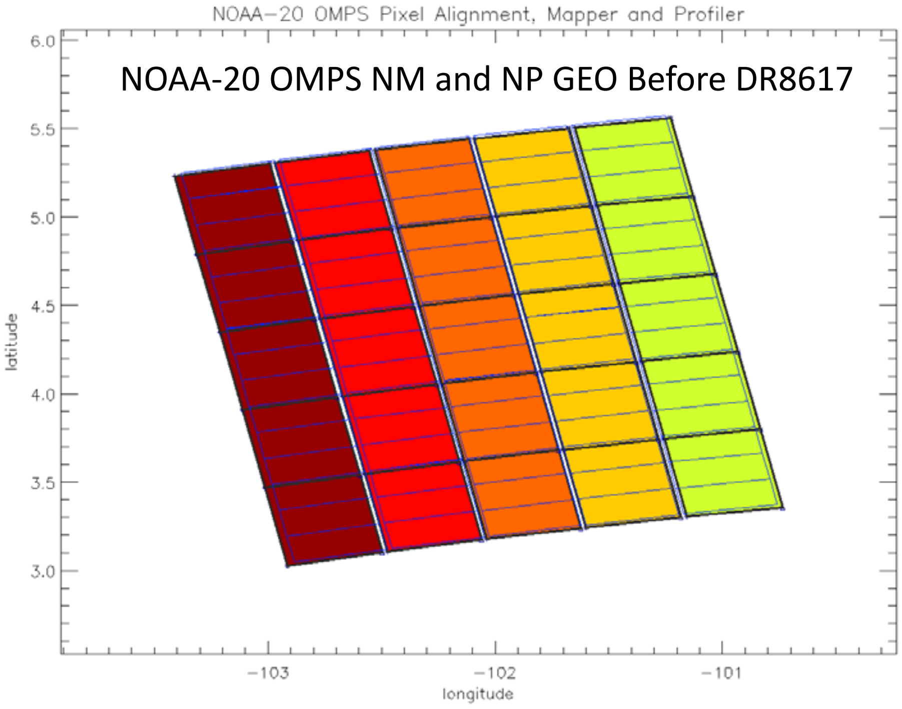


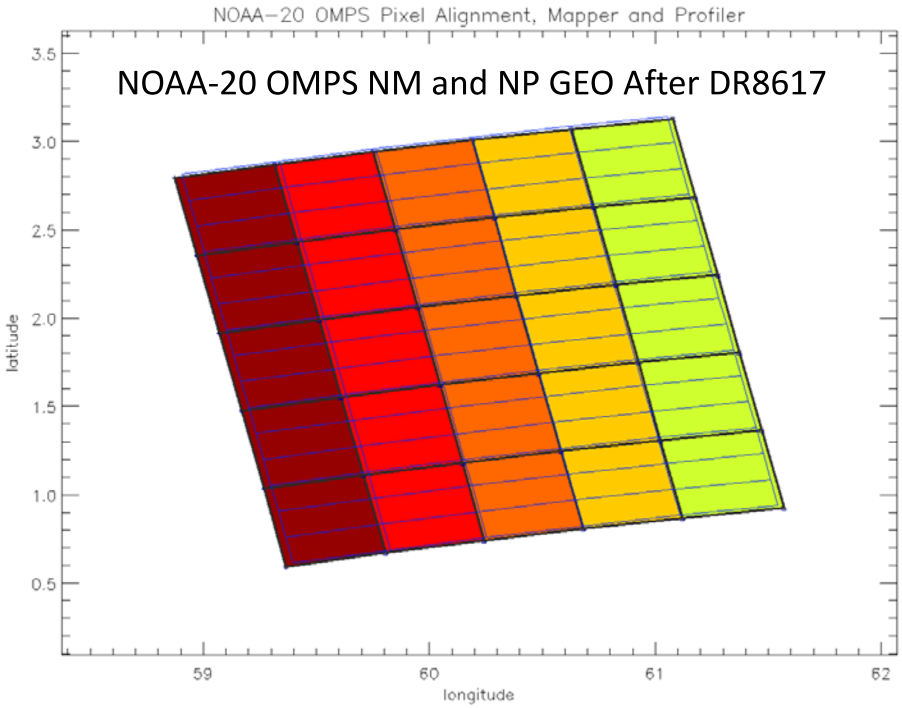
Profile Ozone Error Flags NPP



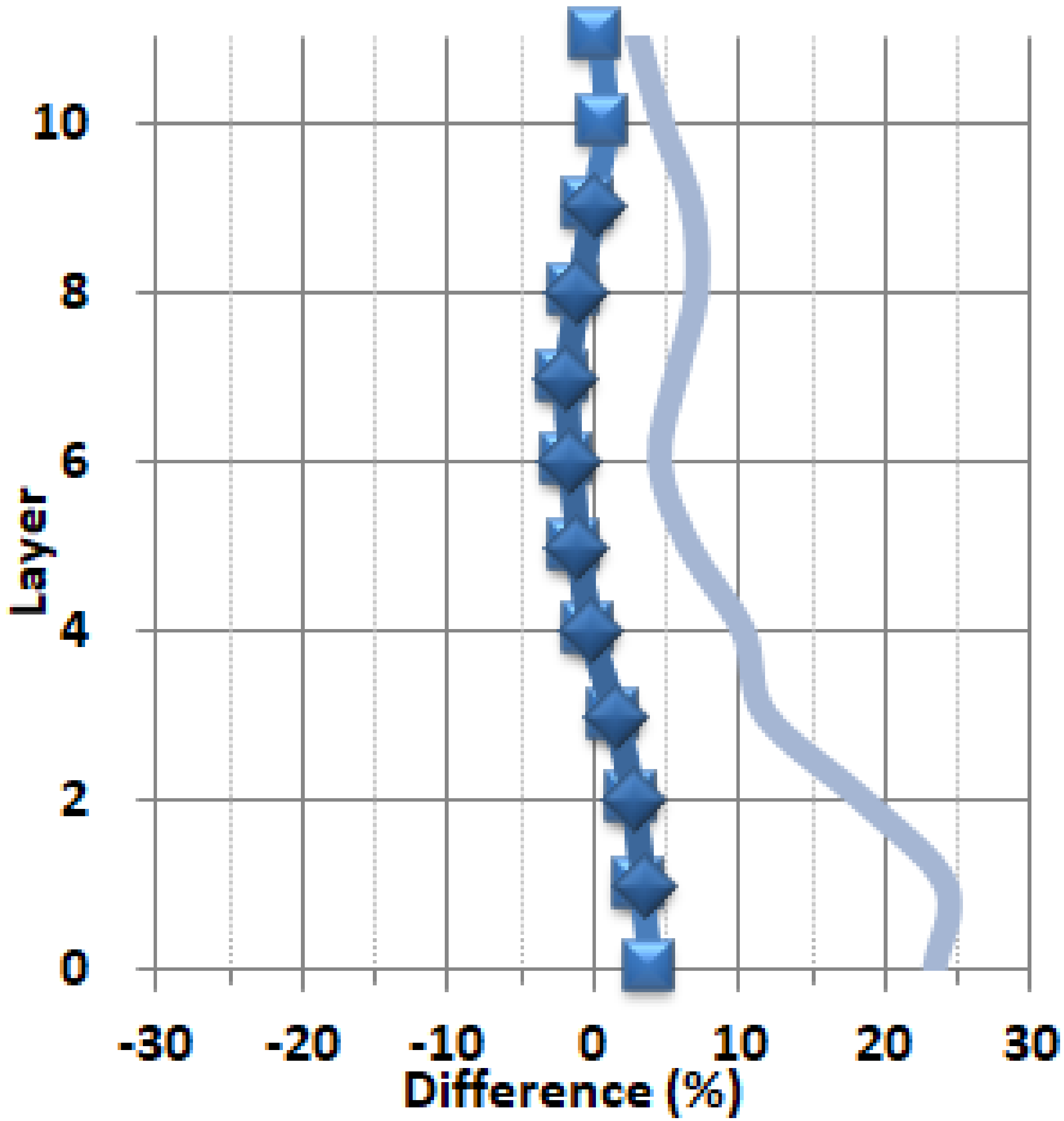
Matchup GEO between OMPS NM and NP

The ground pixel corner geolocation is modified. The first image below shows the ground pixels for one 37-second granule for OMPS-NP and OMPS-TC. The gaps between each FOV are about 2.4km.





S-NPP V8Pro versus Boulder CO Umkehr



V8Pro v3r3 Refinements

A. Dual Adjustment Tables

- Provides Old (Current) and New (Updated) soft calibration tables with the option to interpolate between them to smooth the transition at the request of data assimilation applications. File names will have creation dates.

B. Metadata improvements.

- Additional fields are added to metadata to be consistent with NDE requirements and to provide better information. These include the NDE production site, NDE production environment, and the adjustment table's file name.

C. Area-Weighted FOV Averages

- When the NOAA-20 OMPS NM goes to [10,10,10,10, 5, 10, 5, 10, 10, 10, 10] pixel aggregation, we will want to have area-weighted values computed in the glueware. This refinement provides the code to calculate and use the relative sizes of the FOVs.

D. Remove the use of 340 nm channel for reflectivity.

- Code updates to switch from 340 nm channel to 331 nm channel for some reflectivity calculations for consistency with the NASA V8Pro implementation.

E. Code Fixes

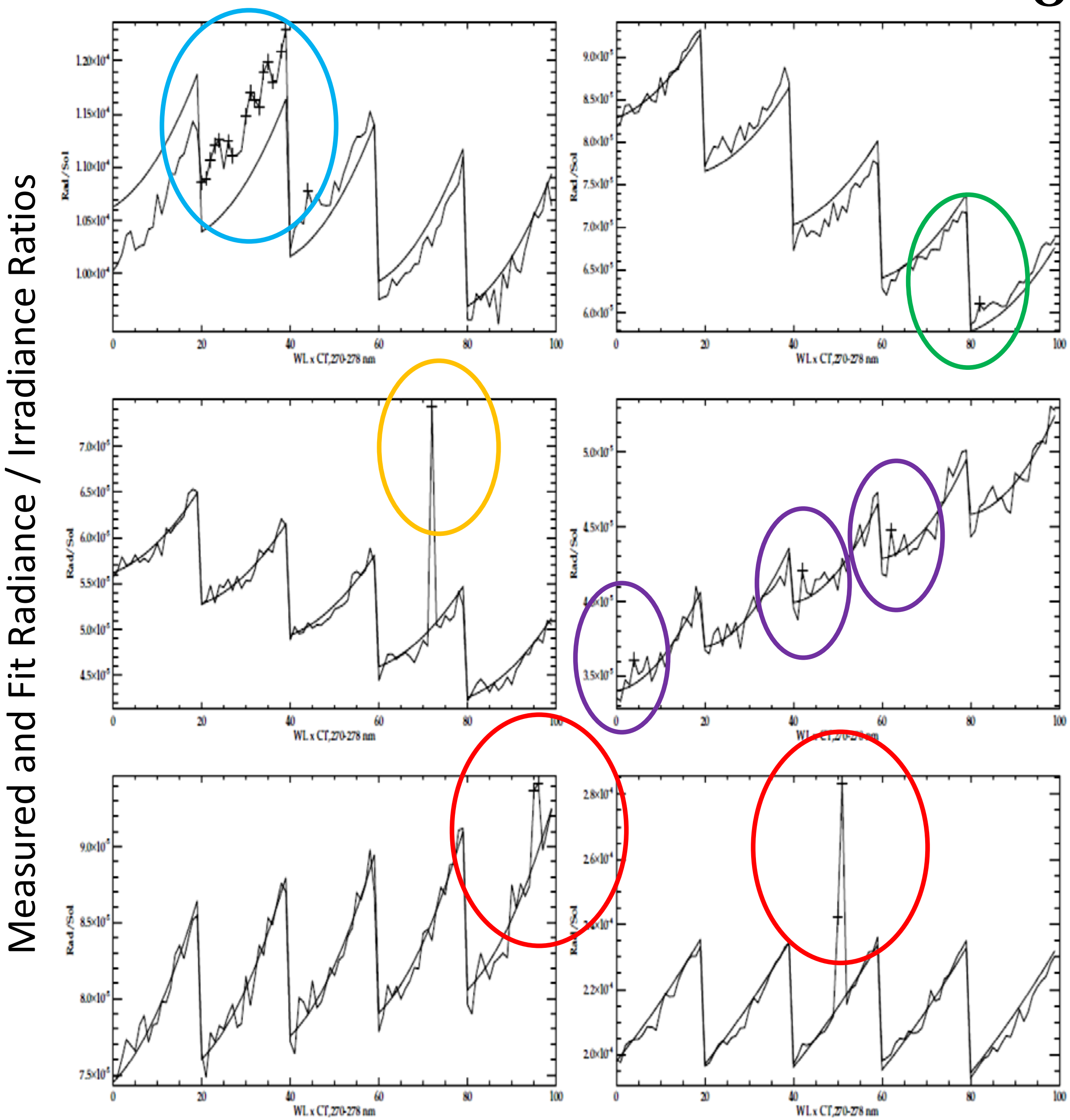
- Averaging Kernels: Change OMPS V8Pro product configuration for the averaging kernels to agree with the SBUV/2 relative response ones.
- Mixing ratio inconsistency in amount and pressure order.
- Terrain Pressure maximum and minimum extended to include Dead Sea and Mt. Everest.
- Descending orbit data are not processed – fixed by changing corner order in Glueware.

F. Changes to handle OMPS NM SDR sizes up to 30 scans x 140 cross-track FOVs per granule.

G. Outlier Detection Filter and Information Concentration (F&IC)

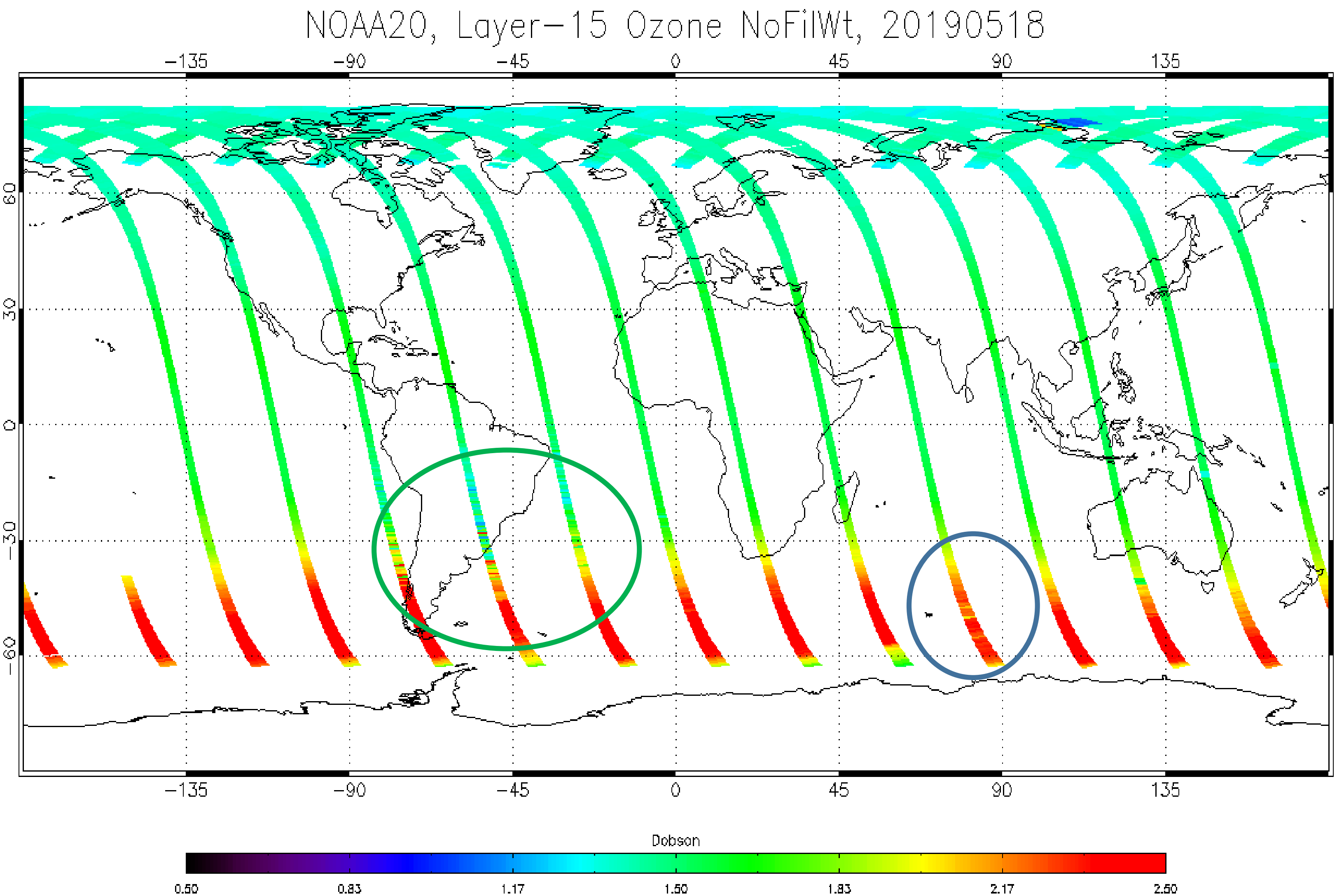
- Implements a combination of median filter and 10- to 12-wavelength polynomial fits of the radiance / irradiance ratios for the shorter ozone profile channels to reduce measurement noise, remove outliers and identify PMCs.

Outlier Detection & Filtering for NOAA-20 OMPS NP

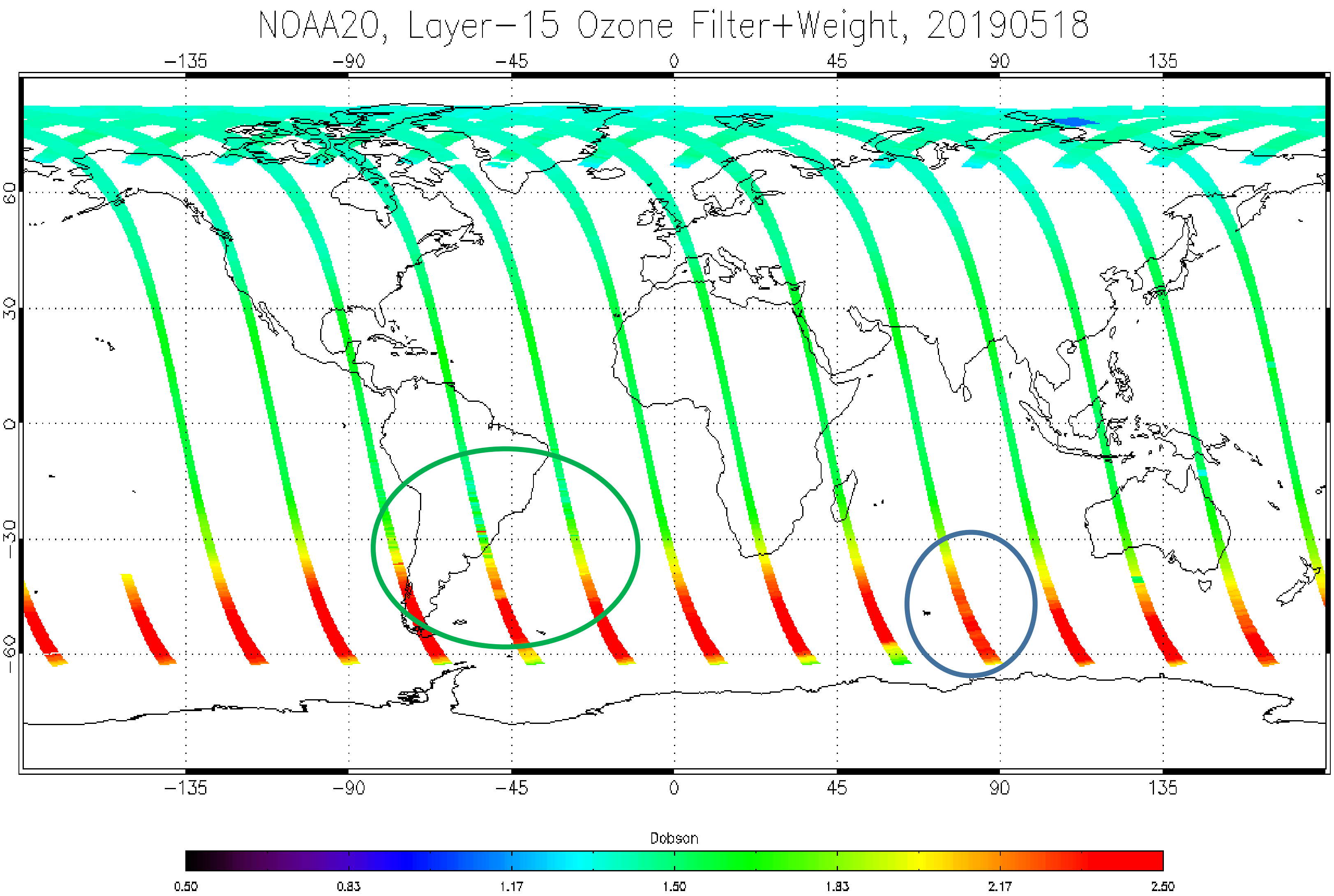


12 Spectral by 5 Cross-track   12 Spectral by 5 Cross-track

Filter with a 4% threshold. A "+" indicates a bad value. Orange - a single spike. Red - two spikes. Purple - three spikes for the same spectral row. These all occurred in the SAA. Blue - high latitude, summer hemisphere, Polar Mesospheric Clouds (PMCs) are present in at least one FOVs. Green - marginal case due to PMCs, or noise, or a charged particle hit in the auroral oval.

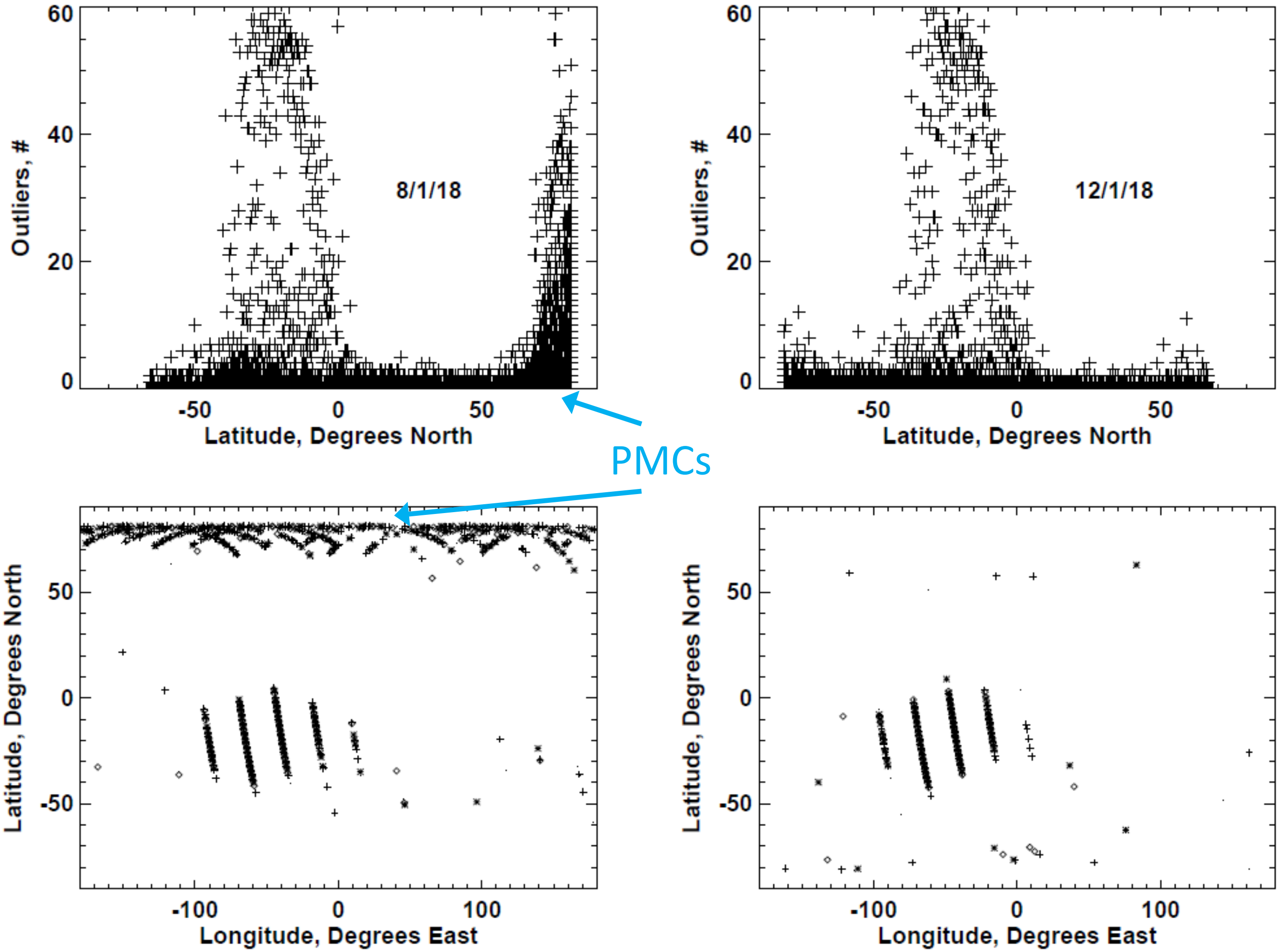


NOAA-20 OMPS V8Pro results for May 18, 2018 without measurements outlier detection and filtering.



NOAA-20 OMPS V8Pro results for May 18, 2018 with measurements outlier detection and filtering.

NOAA-20 2-D Filter Comparison for 274 nm

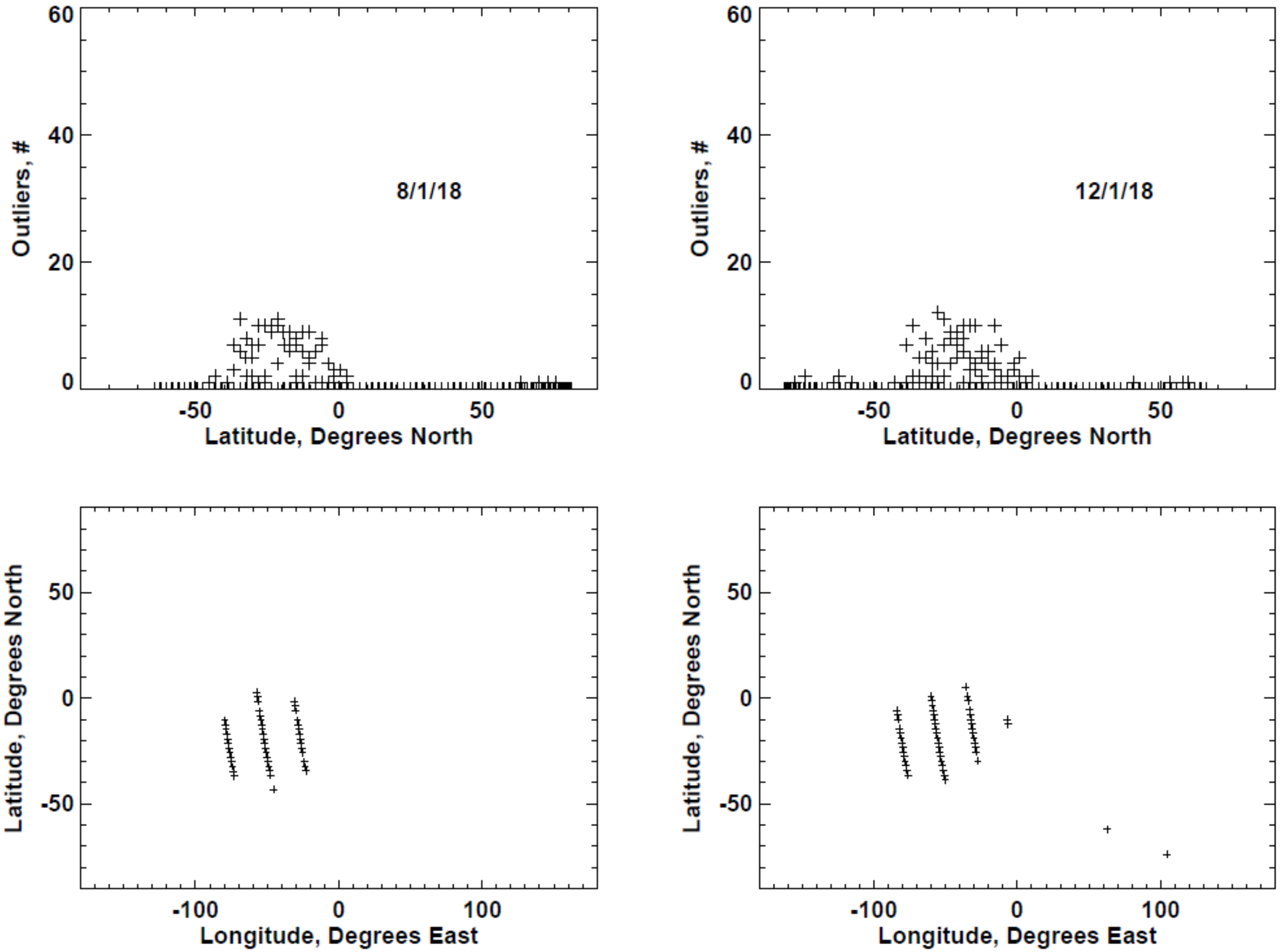


Number and location (for scans with five or more replaced values) of outliers for two days of NOAA-20 OMPS NP SDR data. Twelve wavelength intervals around 273 nm were used and each five cross-track FOV scan was fit with a linear regression using a quadratic model in wavelength and a linear model in cross-track FOV number.

The filter process used an initial difference from a median test of the albedos followed by an iterative removal of terms using the absolute radiance differences from the fit.

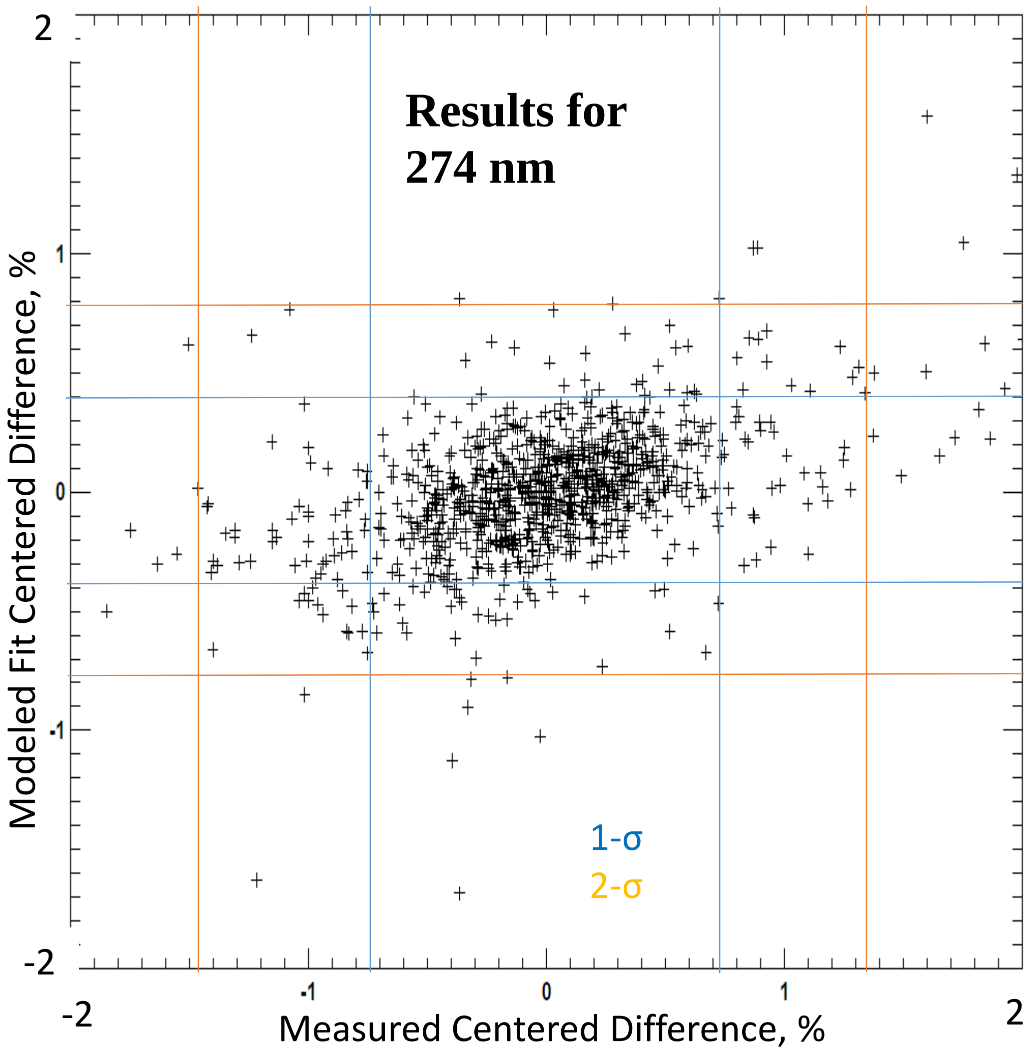
The IDL code to calculate the fits is in the note pages.

S-NPP 2-D Filter Comparison for 274 nm



Number and location (for scans with more two or more replaced outliers) of outliers for two days of S-NPP OMPS NP SDR data. Twelve wavelength intervals around 273 nm were used. The radiance/irradiance ratios for each spectral interval were fit with linear regression using a quadratic model in wavelength.

The filter process used an initial difference from a median test of the albedos followed by and iterative removal of data values using the absolute radiance difference from the fit.



Nearest Neighbor Centered Differences Noise Reduction Estimates

The along-track values at the V8Pro wavelengths for the middle (3rd) scan of five in a granule were compared to the averages of the 2nd and 4th ones. The plot to the left compares the percent differences for the measured results to the those for the model fits for the 274 nm channel.

RMS Differences

nm	ModFit	Measured
253	1.04%	1.73%
274	0.39%	0.73%
283	0.32%	0.47%
288	0.26%	0.46%
292	0.14%	0.27%

The model results show reduced noise for this statistic.

Key Issue for Path Forward from Beta Updates

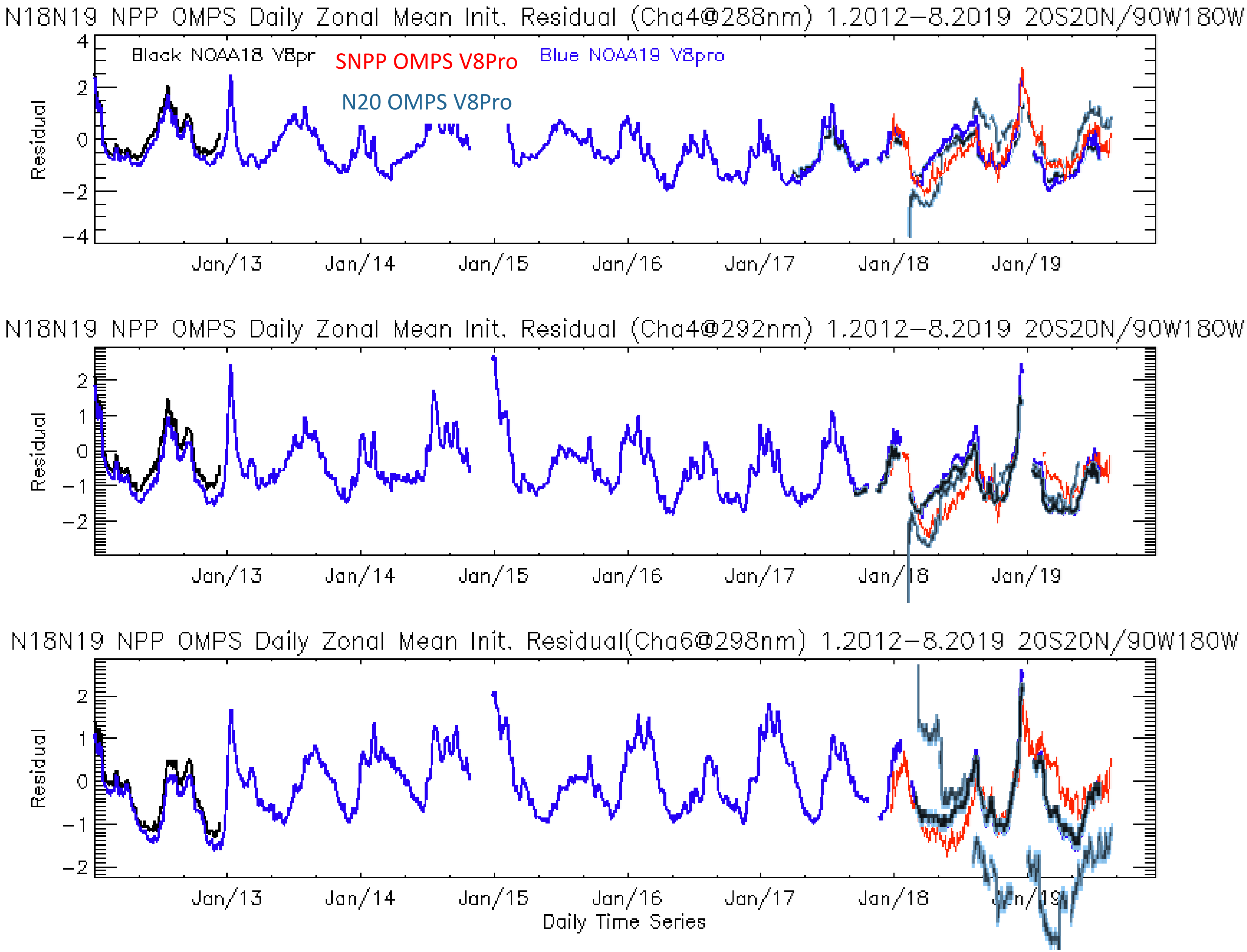
- ADR 8730 New DR. Counts not uniformly distributed for NOAA-20 OMPS NP. This has been traced to discretization errors from the non-linearity correction. A new flight non-linearity was loaded October 19, 2018, and adjustments to the calibration coefficients were implemented at IDPS on December 4, 2018.
- Test data was taken with NOAA-20 OMPS using the new sample tables -- 140 5-pixel for NM and rectangular NP. Tables are under development to make operational 103x15 granule NM SDRs. The SDR team will be requesting that the instrument be switched to the 140 5-pixel mode. We adjusted (v3r3) the V8Pro Glueware to handle the NMmacropixels with

  [10,10,10,10,5,10,5,10,10,10,10] pixels

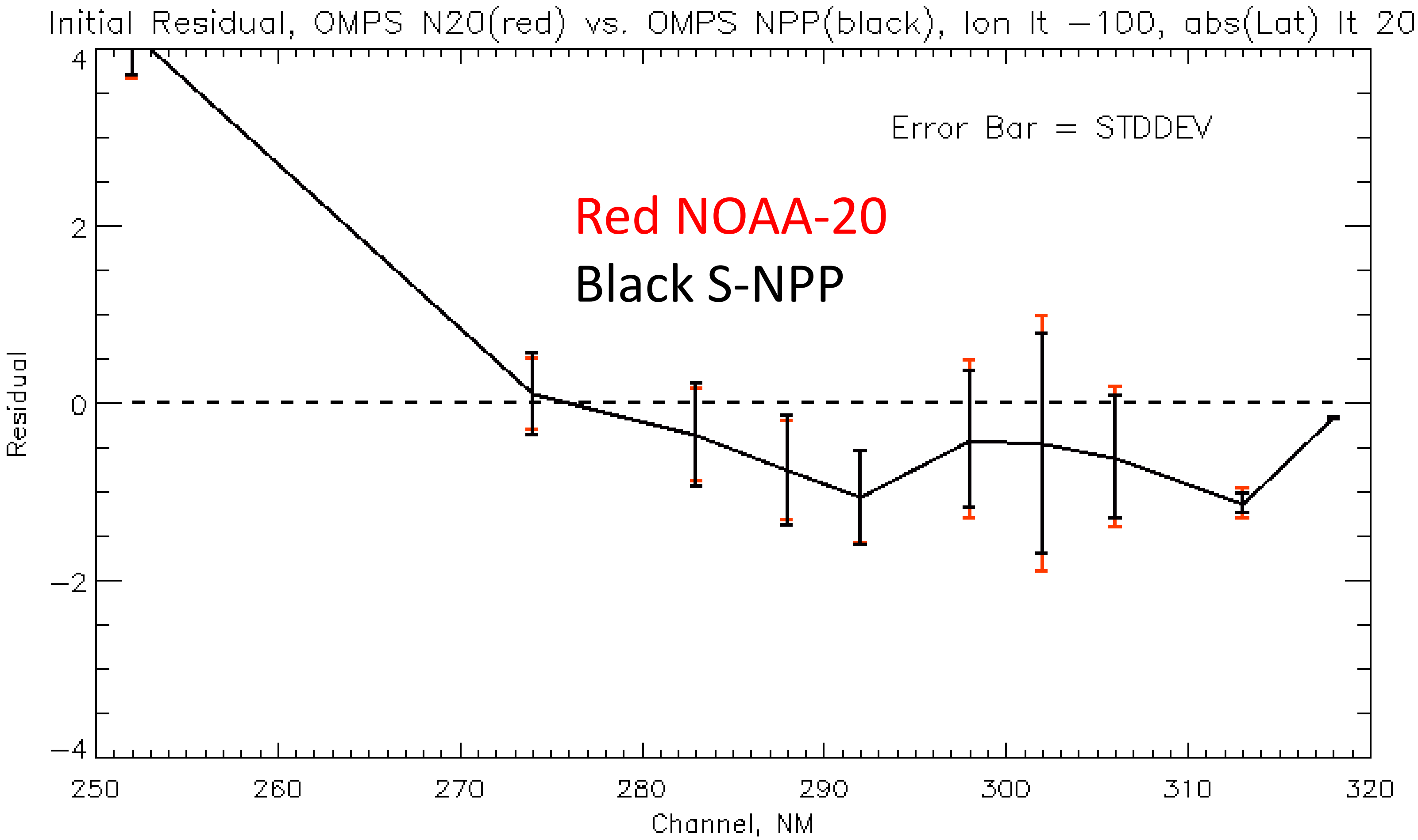
Key SDR changes

- DR8615: Bad NP macropixel calculations for five FOV. Fixed July 2, 2018.
- DR8616: 16-scan granule problem. Fixed September 24, 2018.
- DR8730: Counts not uniformly distributed – Nonlinearity discretization. Fixed December 4, 2018.
- DR8617: FOV mismatch between TC and NP. Fixed April 19, 2019.
- DR8709: Smear transients and negative radiances. Fixed July 25, 2019.
- DR9093: New Stray Light, Calibration Coefficients and Day 1 Solar and Wavelength Scale tables are in testing for NOAA-20 OMPS NM and NP.

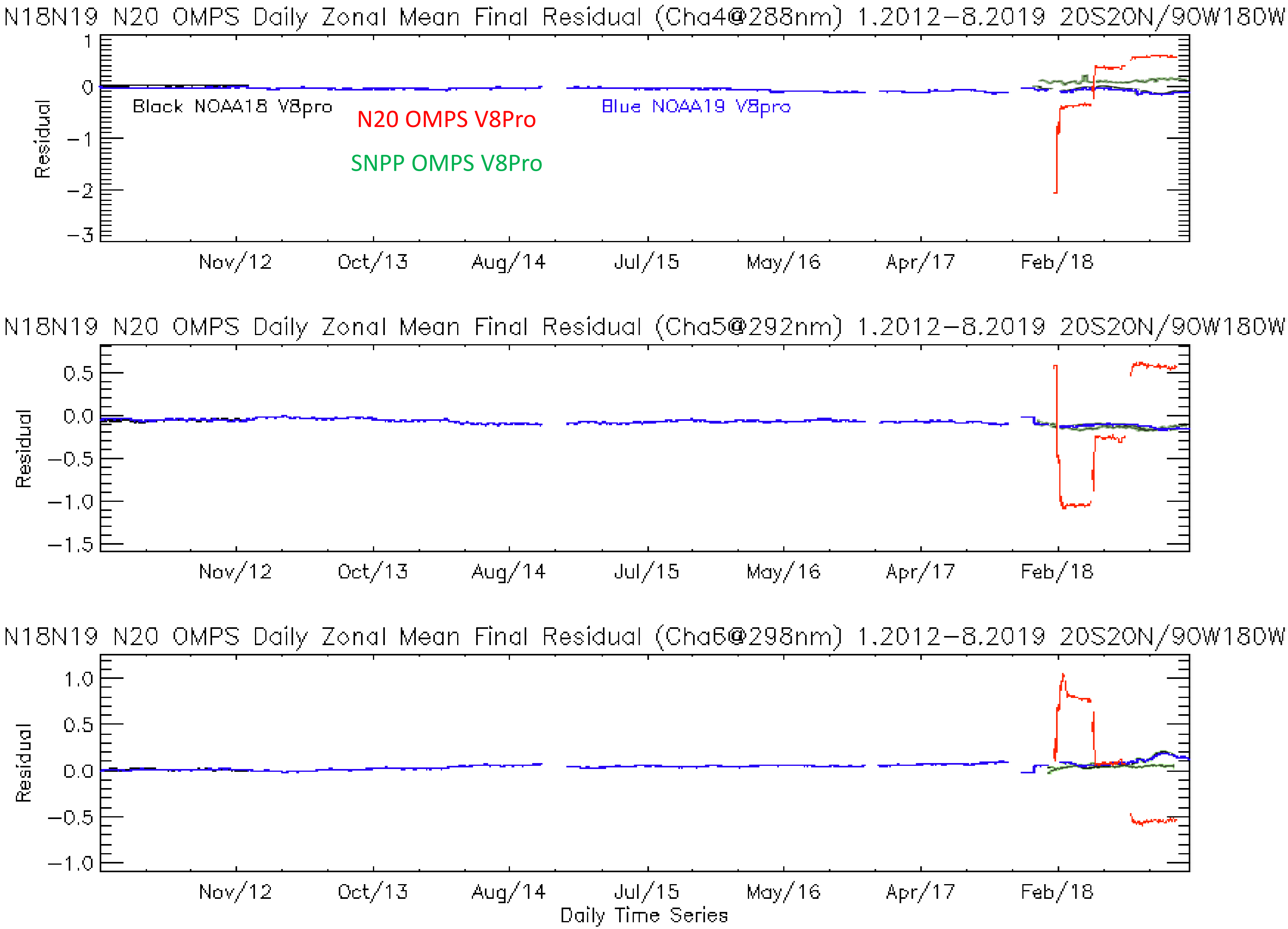
Initial Residuals from NDE V8Pro



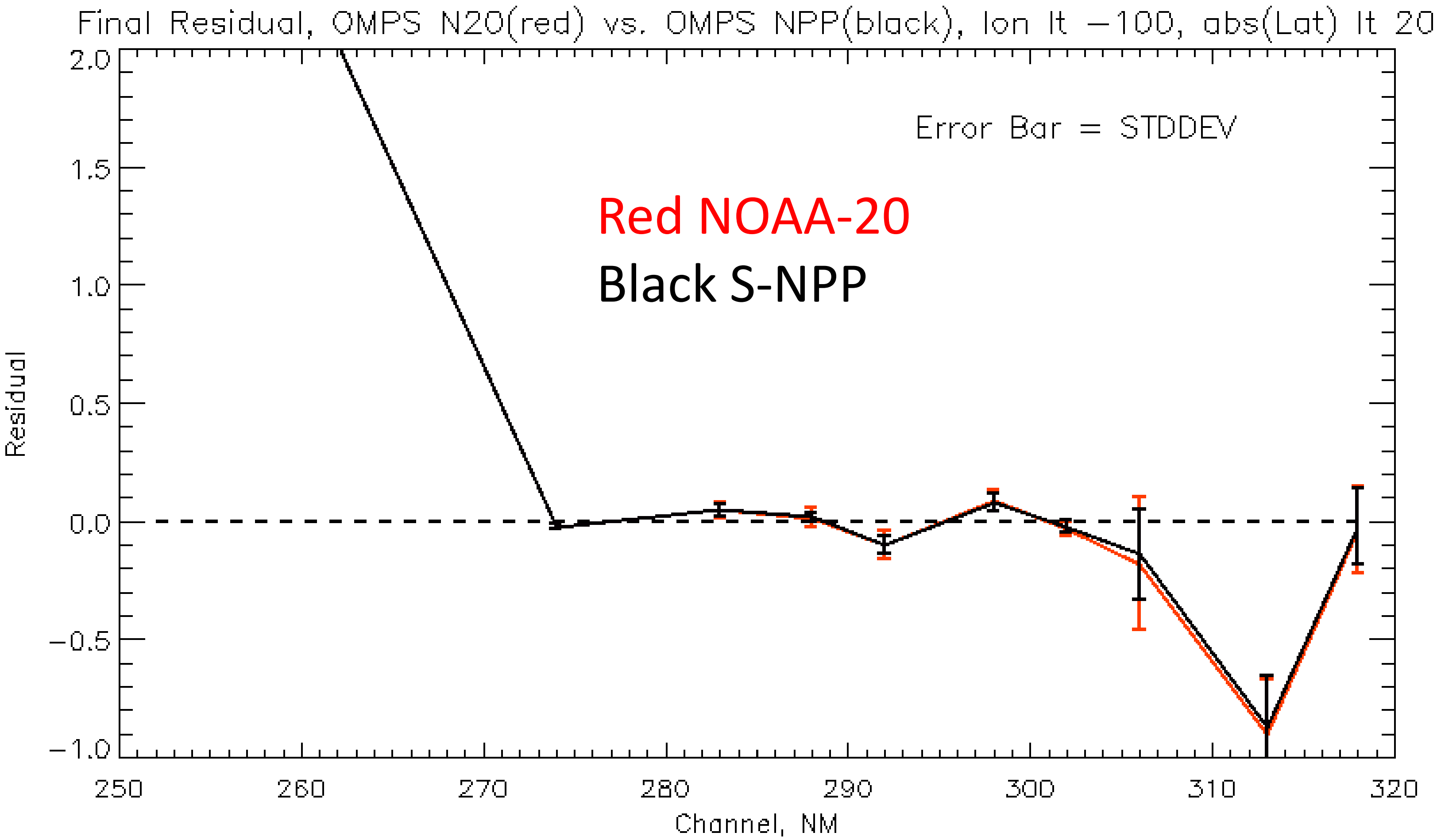
Initial Residuals After Adjustment V8Pro



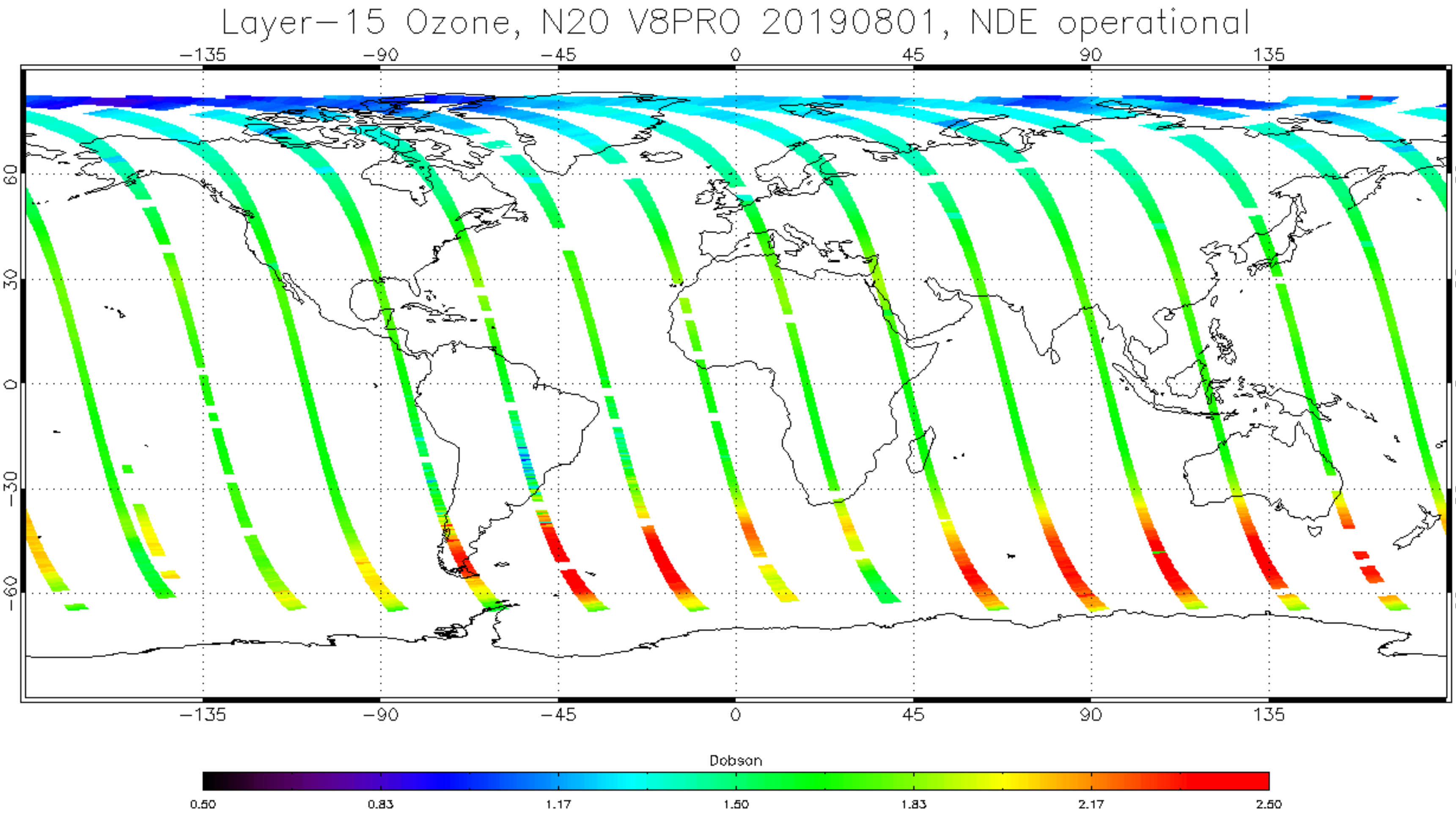
Final residuals from NDE V8Pro



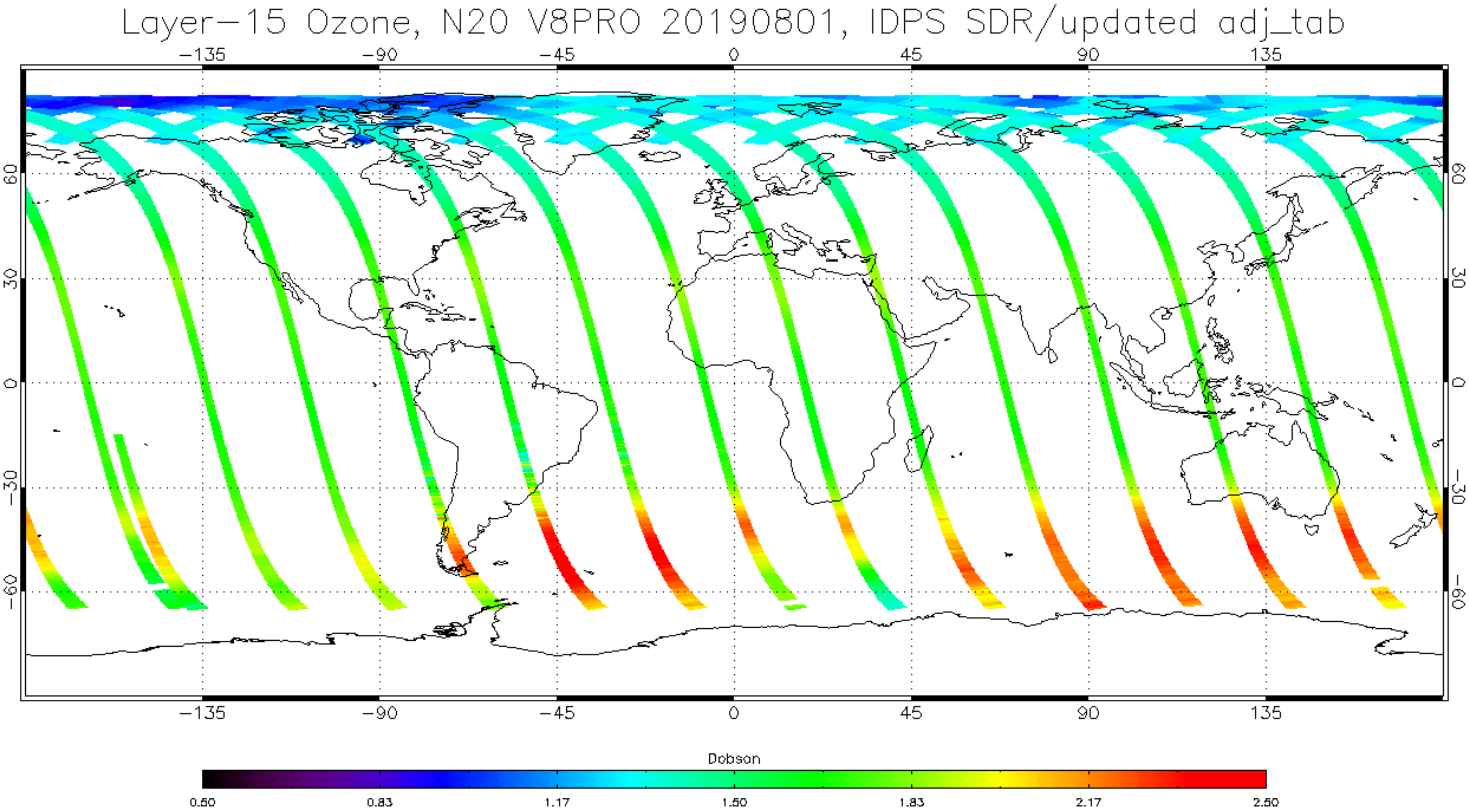
Final Residuals After Adjustment V8Pro



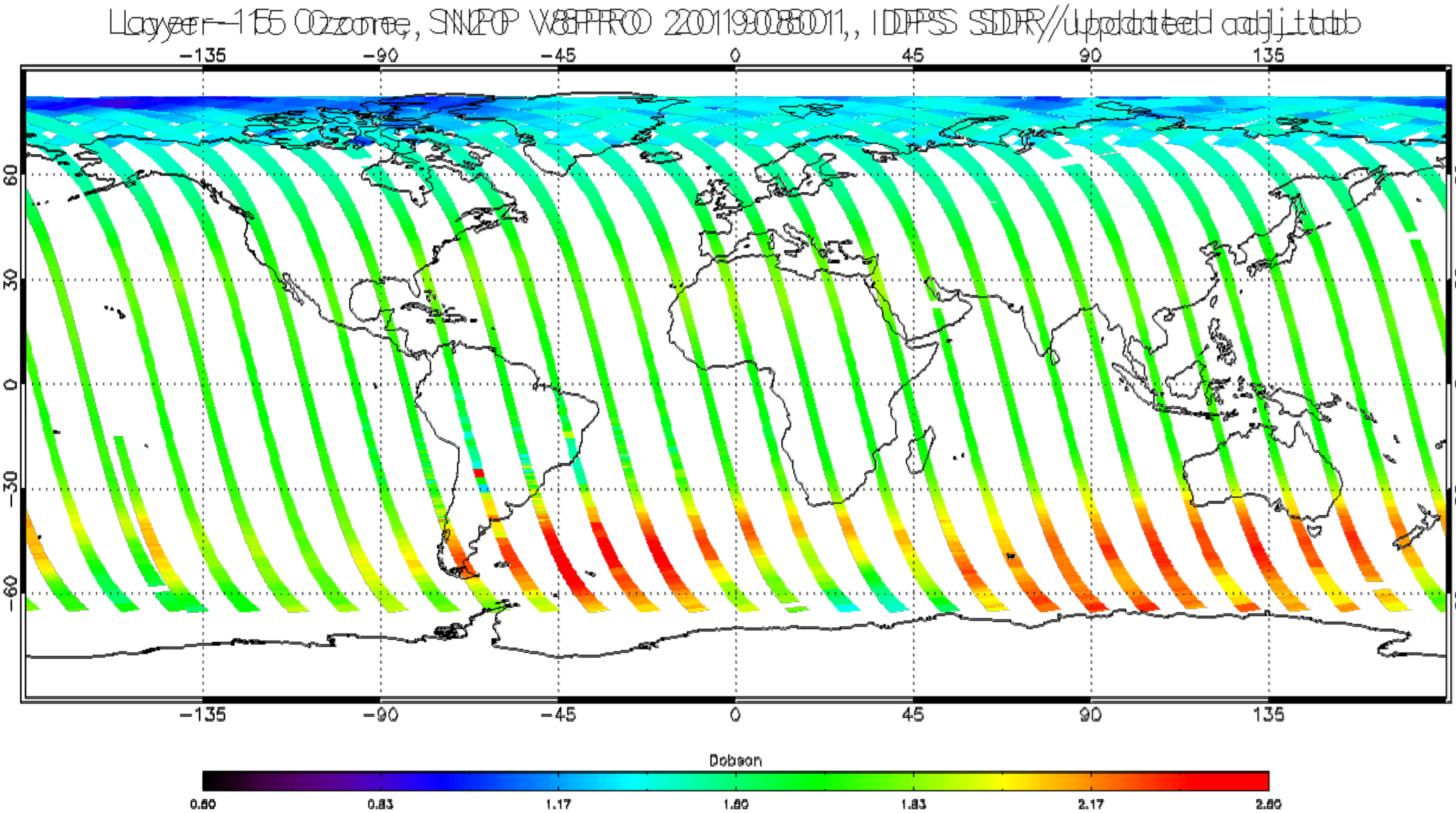
Layer 15 NDE I&T



Layer 15 STAR Offline

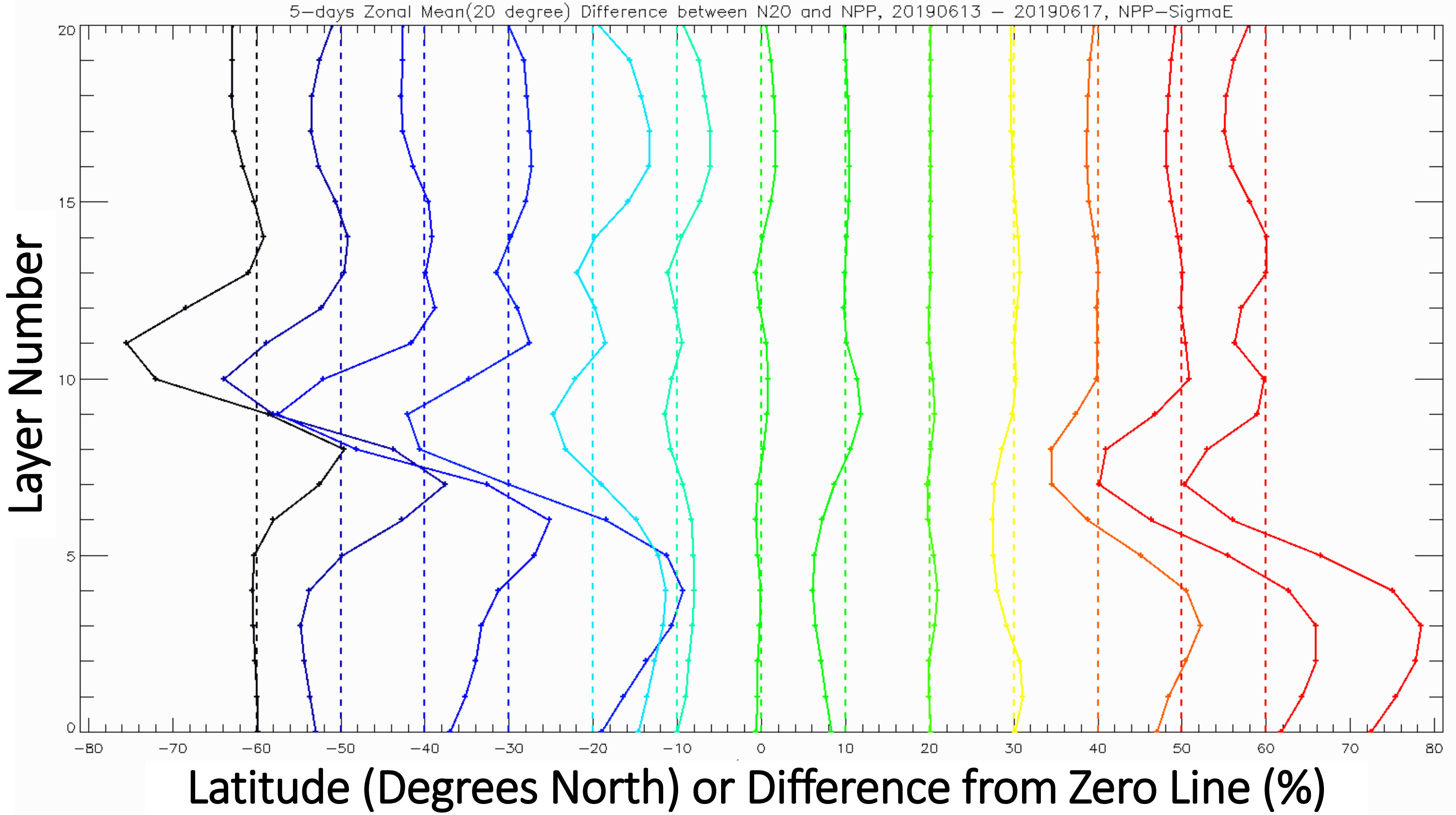


Layer 15 STAR Offline N20 versus NPP

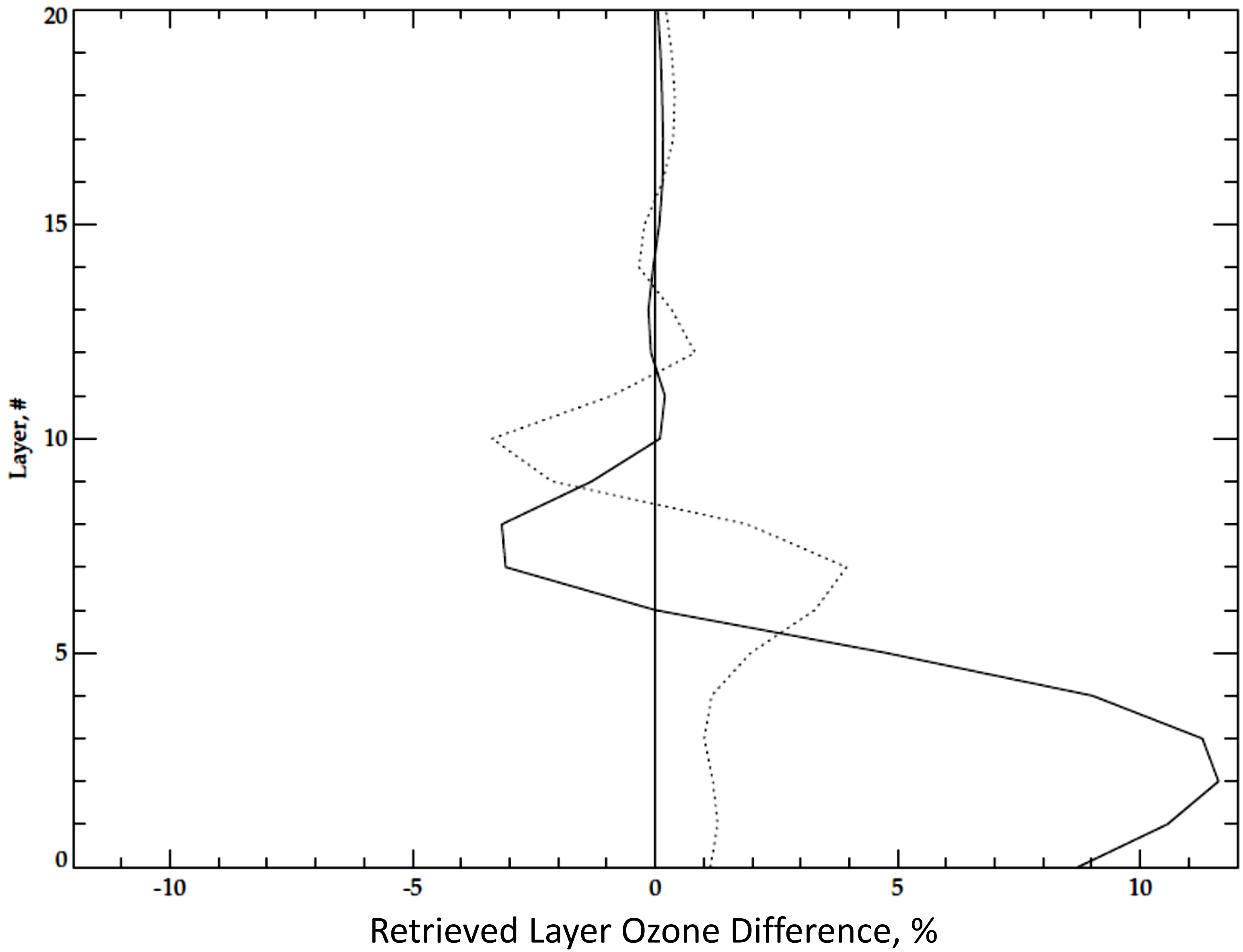


Failure to Force Agreement between NOAA-20 V8Pro and S-NPP V8Pro with Soft Calibration Adjustments

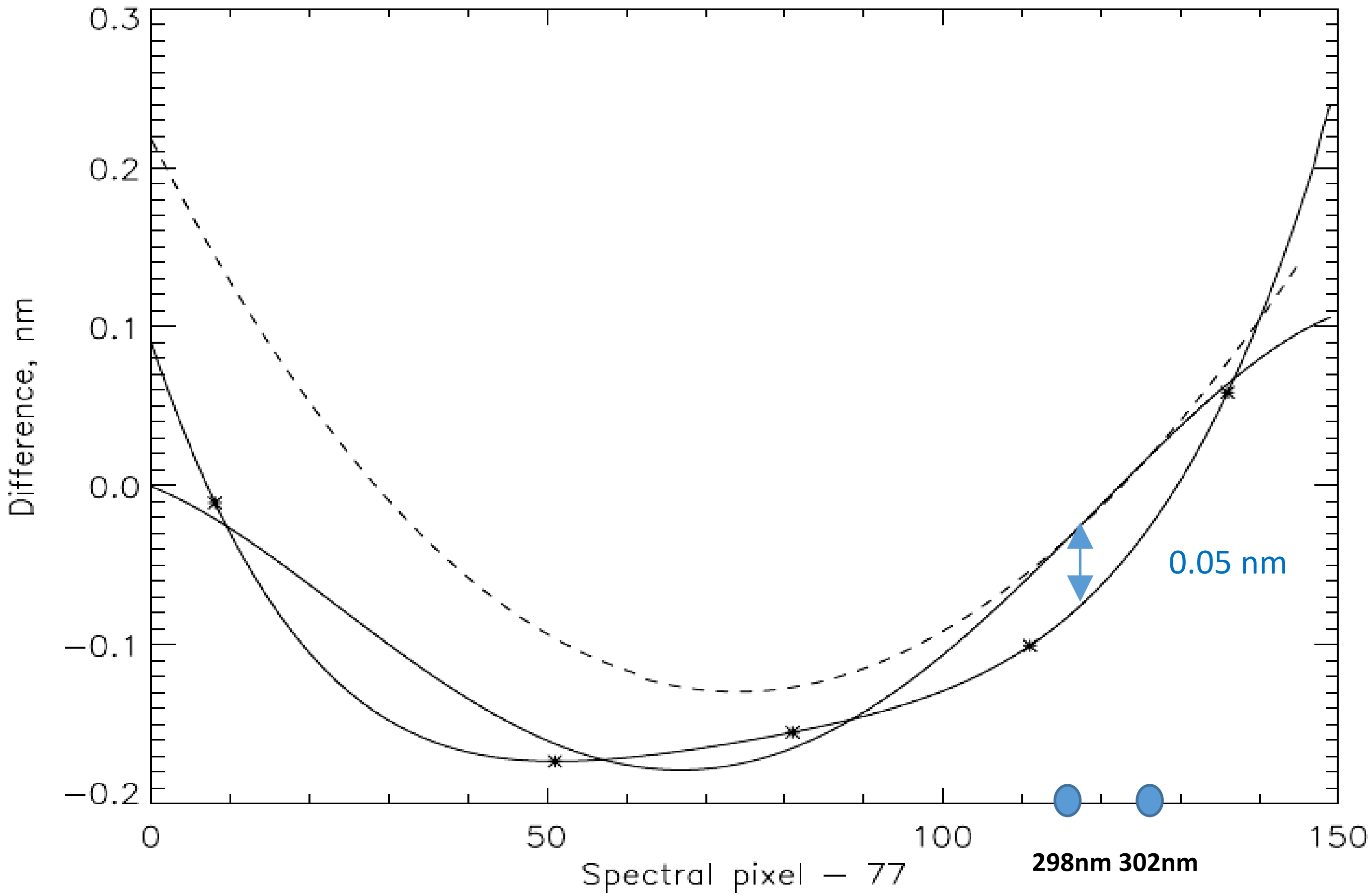
Profile shape differences for S-NPP and NOAA-20 V8Pro Zonal Means after Soft Calibration



Retrieval Sensitivity to 0.04-nm shifts for 302 nm channel [50N-E solid, 50S-E dotted]



Wavelength Scales versus Linear



The S-NPP (dashed) show a close to quadratic wavelength scale. The NOAA-20 (solid) follow a quartic wavelength scale. The solid line without symbols are the NOAA-20 CBC data. **The solid line with symbols (*) are the NOAA-20 CBC data adjusted by the bandpass-weighted average wavelengths**. The symbols in the figure show the locations of the five NOAA-20 pre-launch spectral measurement sets.

Provisional Caveats

- The V8Pro EDR products described in this presentation will not be available from NDE until after delivery and implementation of the latest changes (v3r3).
- The NOAA-20 V8Pro adjustments give good agreement with the S-NPP V8Pro within 20° of latitude of the Equator but the retrievals deviate outside that range.
- The quality of the products will change once the newest SDR tables are delivered and installed at IDPS. We will need to deliver new adjustment tables to obtain agreement between NOAA-20 and S-NPP.
- There is an open question on the OMPS NP SDR wavelength scale. The SDR Team is working on a new wavelength scale but the EDR Team has not demonstrated that it will provide agreement over the full Latitude range.

Processing Environment and Algorithms

- Processing environment and algorithms used to achieve Beta maturity stage:
  - Algorithm version V8Pro_v3r2 at NDE I&T using IDPS I&T SDRs.
  - Same version is used in operations for S-NPP.
  - Version of LUTs used Adjustment from 5/2018.
- Processing environment and algorithms used to achieve Provisional maturity stage:
  - Algorithm version V8Pro_v3r3 proceeding to NDE using IDPS operational SDRs. Will be implemented on the NDE I&T and move to NDE Oprations pending Operational Briefing.
  - Version of LUTs used Adjustment from 6/2019.

Required Algorithm Inputs

- Required Algorithm Inputs
  - Primary Sensor Data
    - NOAA-20 OMPS NM SDR and GEO
    - NOAA-20 OMPS NP SDR and GEO
  - Ancillary Data
    - Ozone and cloud top pressure climatologies.
  - Upstream algorithms
    - OMPS SDR
  - LUTs / PCTs
    - Multiple scattering corrections
    - N-value Adjustment Table

User Feedback

Name	Organization	Application	User Feedback - User readiness dates for ingest of data and bringing data to operations
C. Long, H. Liu	NCEP	O3 Assimilation for NWP, UV Index, and Monitoring.	Will not add NOAA-20 V8Pro BUFR to operational use with current disagreement with S-NPP.

Downstream Product Feedback

Algorithm	Product	Downstream Product Feedback - Reports from downstream product teams on the dependencies and impacts
TOAST	Global Ozone Maps	Currently using S-NPP V8Pro. Will not add NOAA-20 V8Pro with current disagreement.

Risks, Actions, and Mitigations

- Provide updates for the status of the risks/actions identified during the previous maturity review(s); add new ones as needed

Identified Risk	Description	Impact	Action/Mitigation and Schedule
Failure to get agreement	Soft calibration did not resolve differences between S-NPP V8Pro and NOAA-20 V8Pro.	Major	Working with OMPS NP SDR team to investigate wavelength scale accuracy and knowledge.
Implementation	Multiple code and table changes are ready for implementation at NDE.	Major	Working with ASSISTT and NDE to implement new DAP.

Documentations

Science Maturity Check List	Yes / No
ReadMe for Data Product Users (Provisional)	Yes (NOAA-20)
Algorithm Theoretical Basis Document (ATBD)	In revision (V8Pro)
Algorithm Calibration/Validation Plan	Yes (JPSS-1 Ozone)
(External/Internal) Users Manual	In revision (V8Pro)
System Maintenance Manual	In revision (V8Pro)
Peer Reviewed Publications (Demonstrates algorithm is independently reviewed)	Yes (V8Pro)
Regular Validation Reports (at least annually) (Demonstrates long-term performance of the algorithm)	For S-NPP and JPSS Annual and reviews

Check List - Provisional Maturity

Provisional Maturity End State	Assessment
Product performance has been demonstrated through analysis of a large, but still limited (i.e., not necessarily globally or seasonally representative) number of independent measurements obtained from select locations, periods, and associated ground truth or field campaign efforts.	Product agreement with S-NPP V8Pro has only been obtained for the Equatorial zone.
Product analysis is sufficient to communicate product performance to users relative to expectations (Performance Baseline).	Differences as a function of layer and latitude have been quantified.
Documentation of product performance exists that includes recommended remediation strategies for all anomalies and weaknesses. Any algorithm changes associated with severe anomalies have been documented, implemented, tested, and shared with the user community.	The TIM presentation on V8Pro refinements described motivations and changes.
Product is ready for operational use and for use in comprehensive cal/val activities and product optimization.	With limits as noted in ReadMe.

Path Forward & Conclusion

- Working with SDR Team to resolve failure to obtain agreement between S-NPP V8Pro and NOAA-20 V8Pro.
- Working with ASSISTT, OSPO and NDE to complete implementation of new code, table and document changes
- Team recommends provisional maturity for V8Pro EDR
    - Product performance relative to S-NPP is only good in the Tropics.
    - Feedback from users may help to resolve S-NPP and NOAA-20 differences.

Backup and previous presentations

Working with NDE

- There are two sources of products from NDE, the operational string and the integration and testing string. They run new revisions on the I&T before moving them to operations and they are currently only running the NOAA-20 on the I&T. The I&T at NDE uses the I&T from IDPS.
- We also make products at STAR either to compare with NDE or because NDE has not put in the newest revisions or because we want to run then with reprocessed SDRs. The NOAA-20 V8TOz spatial resolution also changes over time.
- The SDRs are updated as we find problems. For example the S-NPP OMPS NM has a new stray light correction as of the middle of last month, and NOAA-20 OMPS NP will have revised non-linearity and calibration tables in a month of so.
- The EDRs have soft calibration adjustments and these are updated either as we make comparisons on the path to validation or when the SDRs have changed. There is a time lag for the EDR adjustments after and SDR change
- There are satellite, version and revision numbers in the files names that track some of this.
- For examples,
- v3r0_npp is Revision 0 for S-NPP
- and
- v3r1_j01 is Revision 1 for NOAA-20

WHAT DOES IT TAKE TO MAKE NOAA-20 OMPS NP V8PRO AGREE WITH S-NPP OMPS NP V8PRO?

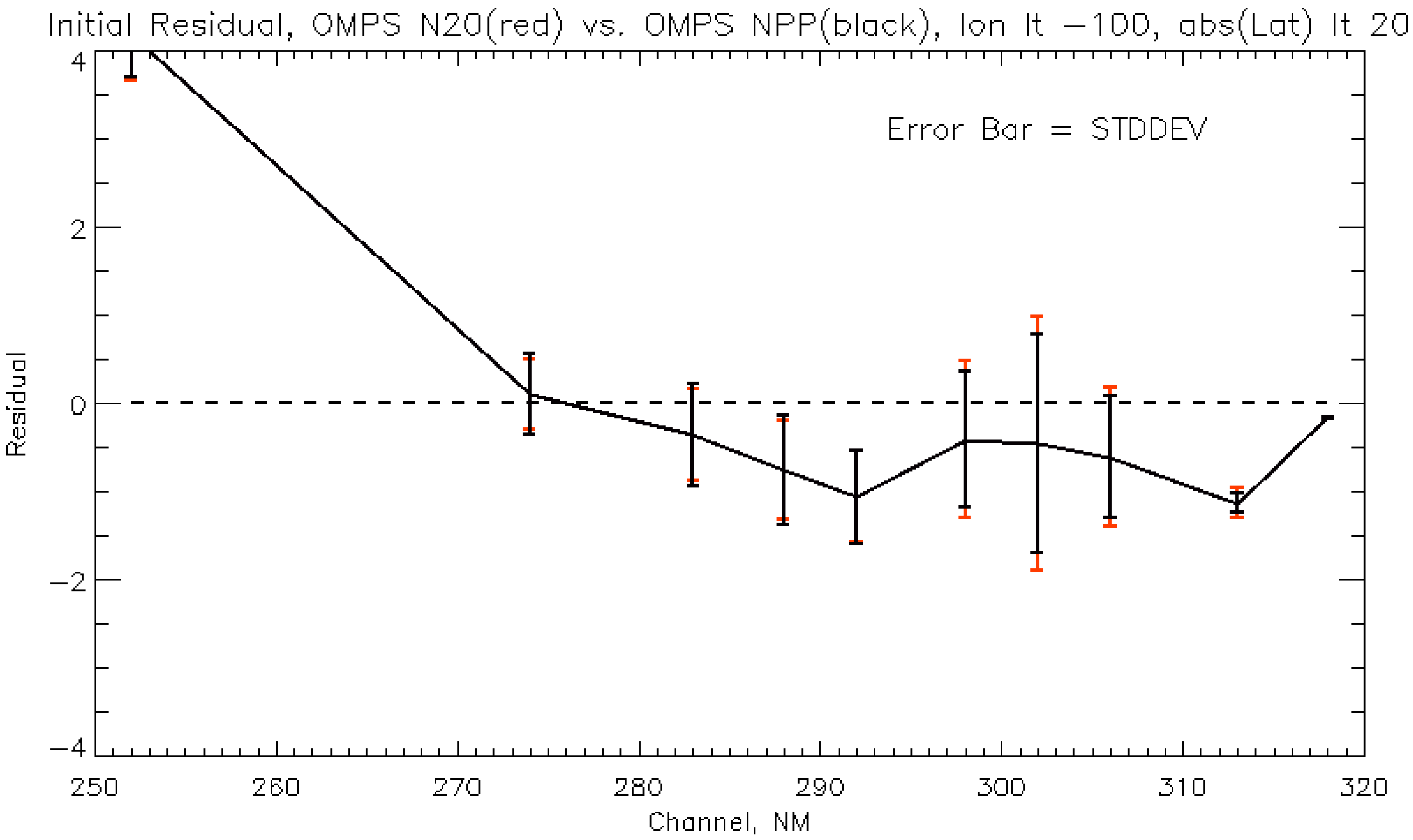
Z. Zhang and L. Flynn

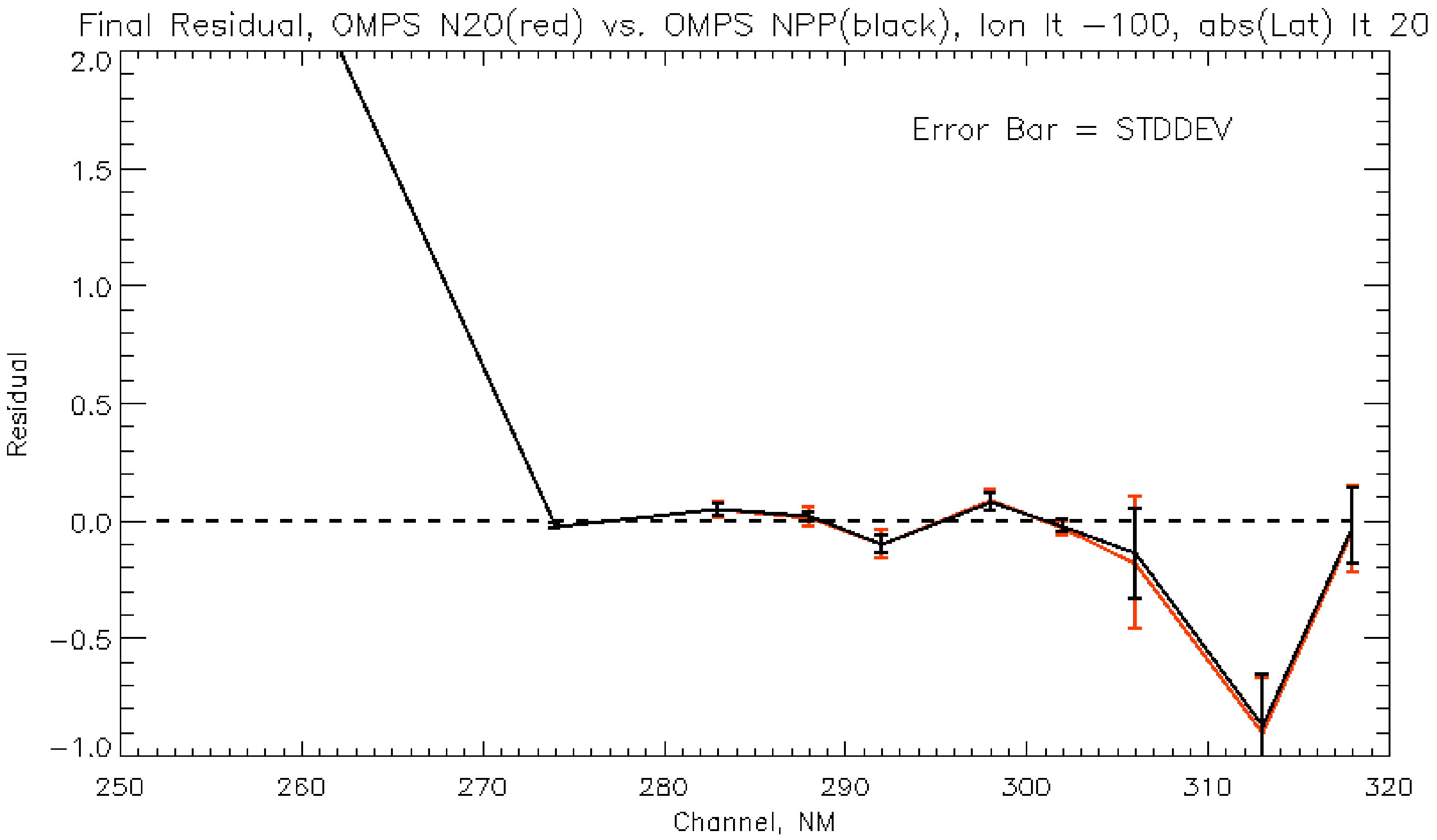
DR Path Forward

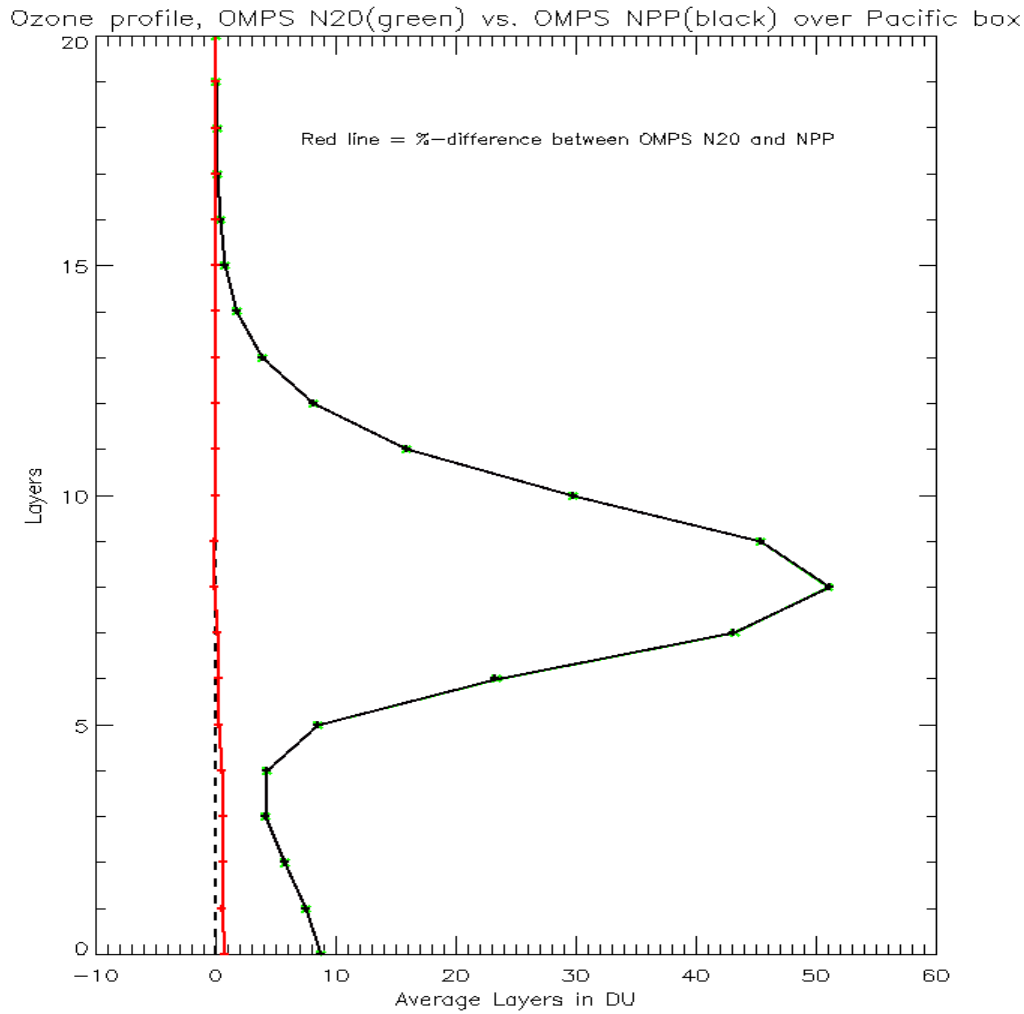
- Confirm better performance of S-NPP OMPS Versus NOAA-19 SBUV/2
- Check wavelength scale for NOAA-20 OMPS NP Solar measurements
  - Construct proxies from high resolution reference solar. Is Mg II in the correct place?
- Compare to S-NPP OMPS NP Solar wavelength scale
- Apply first moment bandpass offsets for NOAA-20 to wavelength scale (both BATC ground-based and Dichroic/QE). Implement new re-centered table.
- Reverse engineer wavelength shifts using sensitivities and retrievals
- Compare TropoMI to S-NPP OMPS
- Compare wavelength scales and solar for NASA Best to NOAA Current (They appear to match well.)
  - Improve understanding of NASA analysis and adjustments
  - Are the goodness of fit results for Solar versus proxy similar for S-NPP and NOAA-20? Do we see the current wavelength scale inaccuracies?
- Does BATC analysis create jumps in dichroic region? Counts vs. Radiances?

5-days mean over pacific box, after soft-calibration with NPP-SigmaE

npp/OMPS reflec is:	0.215217
n20/OMPS reflec is:	0.215216
npp/OMPS aerosl is:	0.374734
n20/OMPS aerosl is:	0.381764
npp/OMPS stp1oz is:	265.323
n20/OMPS stp1oz is:	265.323
npp/OMPS stp2oz is:	263.599
n20/OMPS stp2oz is:	263.598
npp/OMPS stp3oz is:	262.503
n20/OMPS stp3oz is:	262.483
npp/OMPS totpro is:	262.414
n20/OMPS totpro is:	262.611

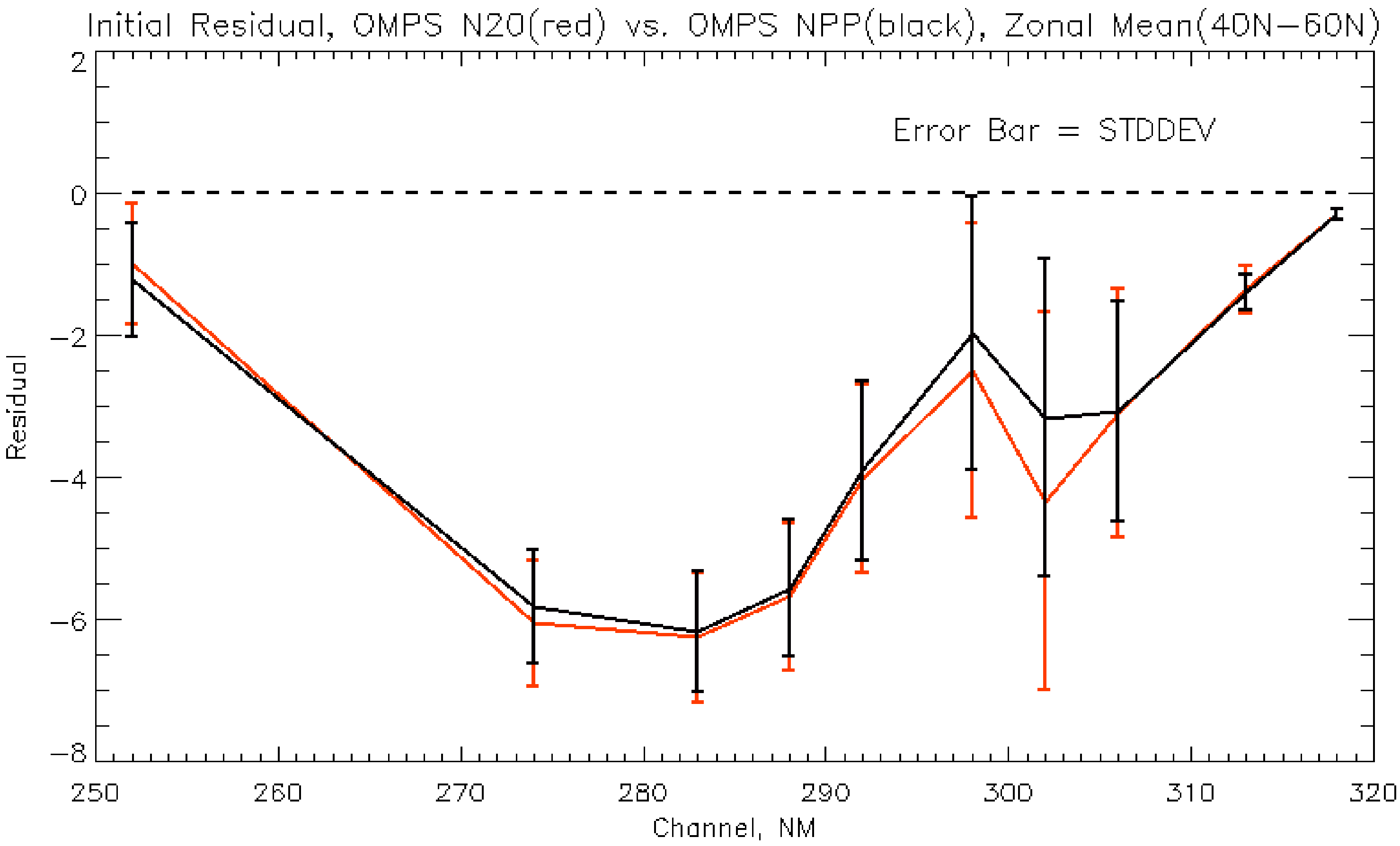

Initial Residual, OMPS N20(red) vs. OMPS NPP(black), lon lt −100, abs(Lat) lt 20
Error Bar = STDDEV
Residual
4
2
0
−2
−4
250
260
270
280
290
300
310
320
Channel, NM

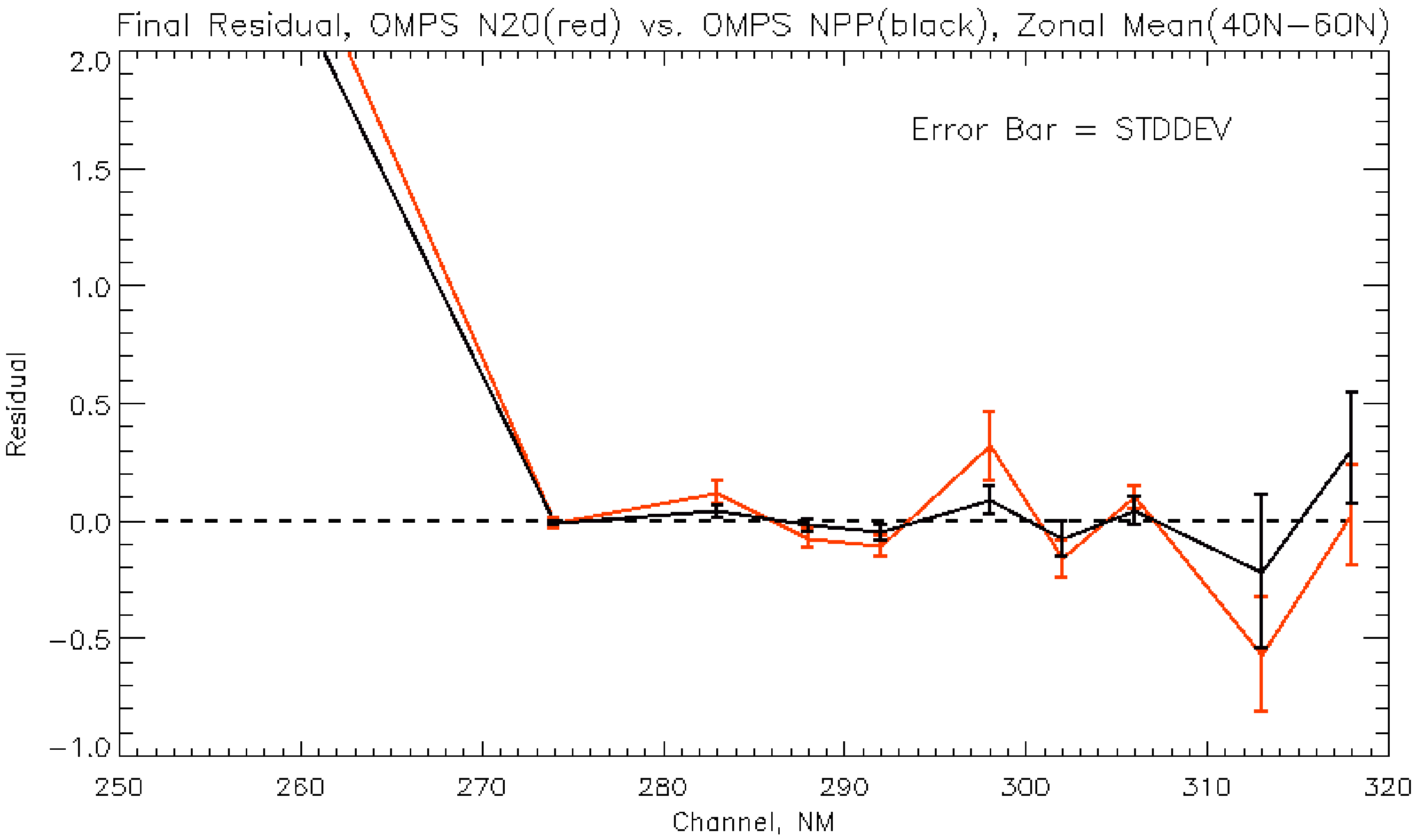

Final Residual, OMPS N20(red) vs. OMPS NPP(black), lon lt −100, abs(Lat) lt 20
Error Bar = STDDEV
Residual
Channel, NM
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
250
260
270
280
290
300
310
320

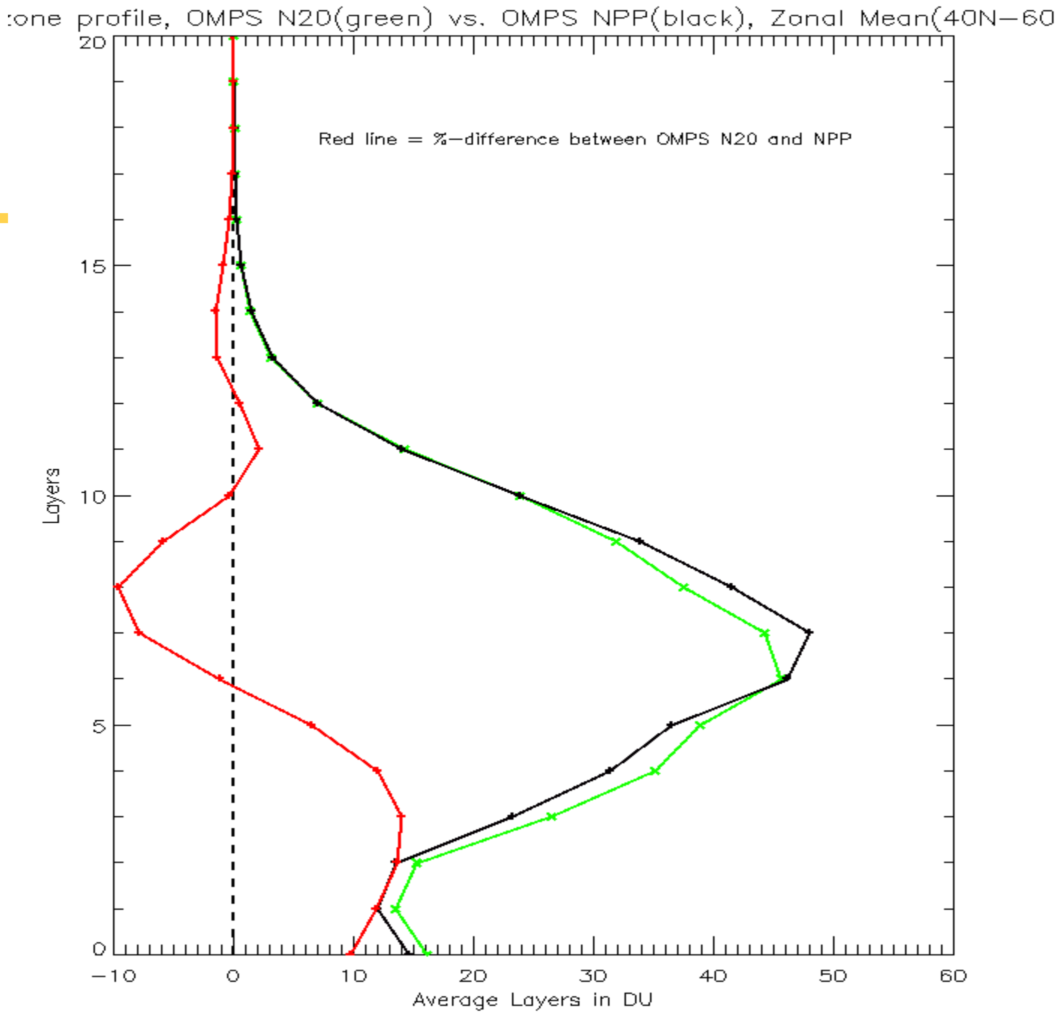

Ozone profile, OMPS N20(green) vs. OMPS NPP(black) over Pacific box
Red line = %-difference between OMPS N20 and NPP
Layers
Average Layers in DU
20
15
10
5
0
-10
0
10
20
30
40
50
60

5-days Zonal mean(40N-60N), after soft-calibration with J01-SigmaE

npp/OMPS reflec is:	0.349198
n20/OMPS reflec is:	0.348413
npp/OMPS aerosl is:	0.472588
n20/OMPS aerosl is:	0.539364
npp/OMPS stp1oz is:	356.133
n20/OMPS stp1oz is:	355.487
npp/OMPS stp2oz is:	355.287
n20/OMPS stp2oz is:	354.669
npp/OMPS stp3oz is:	353.512
n20/OMPS stp3oz is:	352.647
npp/OMPS totpro is:	351.547
n20/OMPS totpro is:	355.543


Initial Residual, OMPS N20(red) vs. OMPS NPP(black), Zonal Mean(40N−60N)
Error Bar = STDDEV
Residual
Channel, NM
2
0
−2
−4
−6
−8
250
260
270
280
290
300
310
320

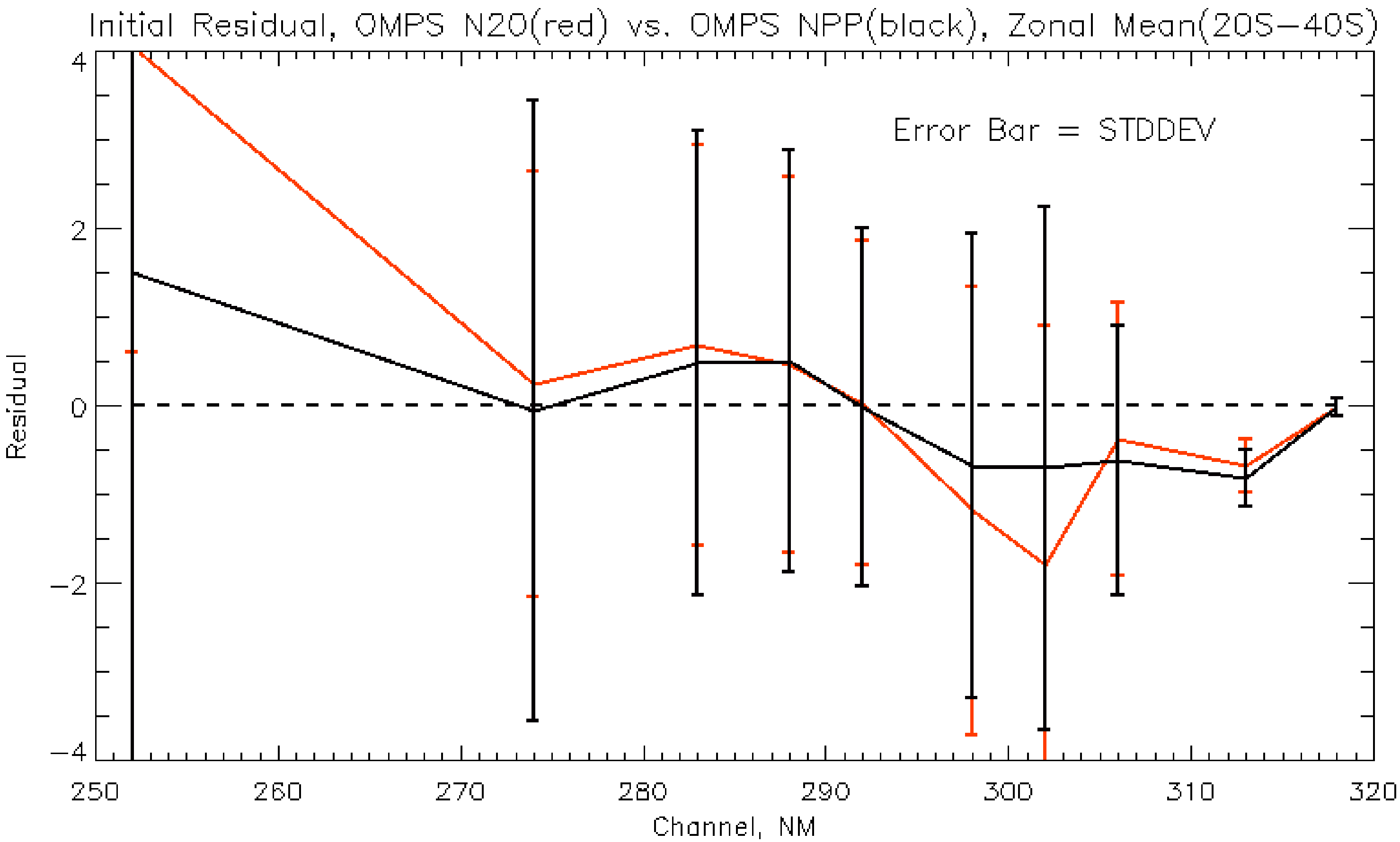

Final Residual, OMPS N20(red) vs. OMPS NPP(black), Zonal Mean(40N−60N)
Error Bar = STDDEV
Residual
Channel, NM
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
250
260
270
280
290
300
310
320



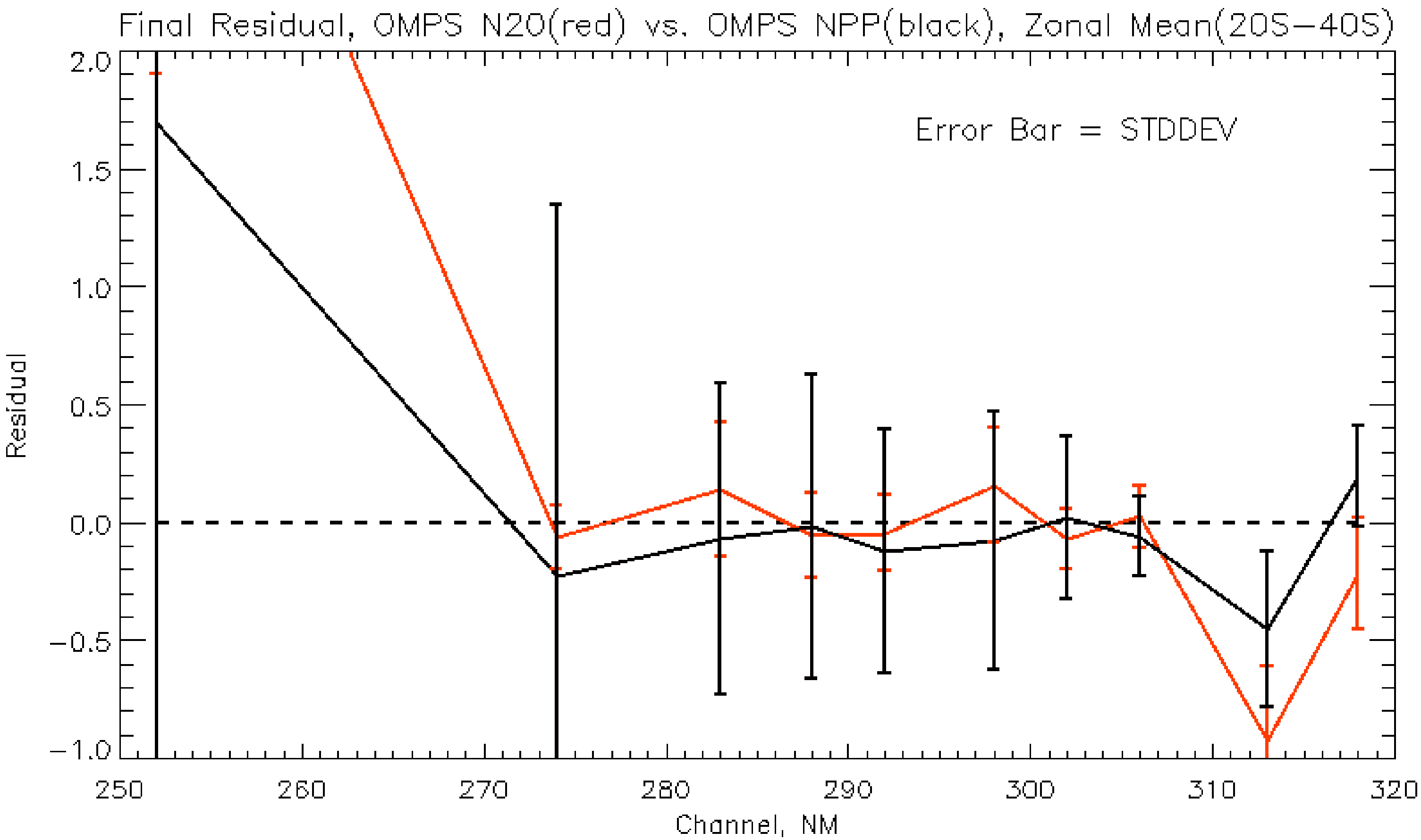
:one profile, OMPS N20(green) vs. OMPS NPP(black), Zonal Mean(40N–60
Red line = %–difference between OMPS N20 and NPP
Layers
Average Layers in DU
20
15
10
5
0
–10
0
10
20
30
40
50
60

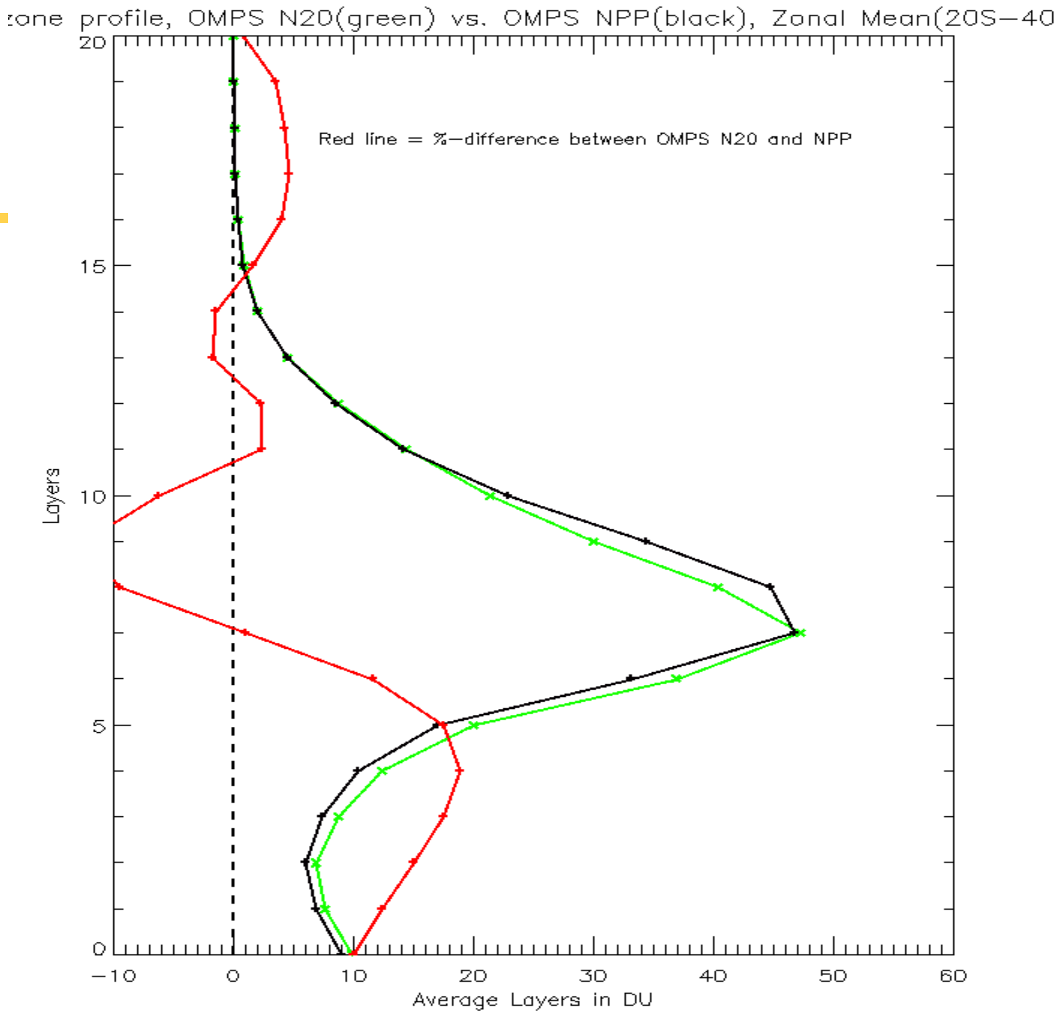
5-days Zonal mean(20S-40S), after soft-calibration with J01-SigmaE

npp/OMPS reflec is:	0.246555
n20/OMPS reflec is:	0.254965
npp/OMPS aerosl is:	-0.441741
n20/OMPS aerosl is:	-0.330401
npp/OMPS stp1oz is:	272.638
n20/OMPS stp1oz is:	271.120
npp/OMPS stp2oz is:	271.597
n20/OMPS stp2oz is:	270.126
npp/OMPS stp3oz is:	272.397
n20/OMPS stp3oz is:	270.736
npp/OMPS totpro is:	268.885
n20/OMPS totpro is:	272.548

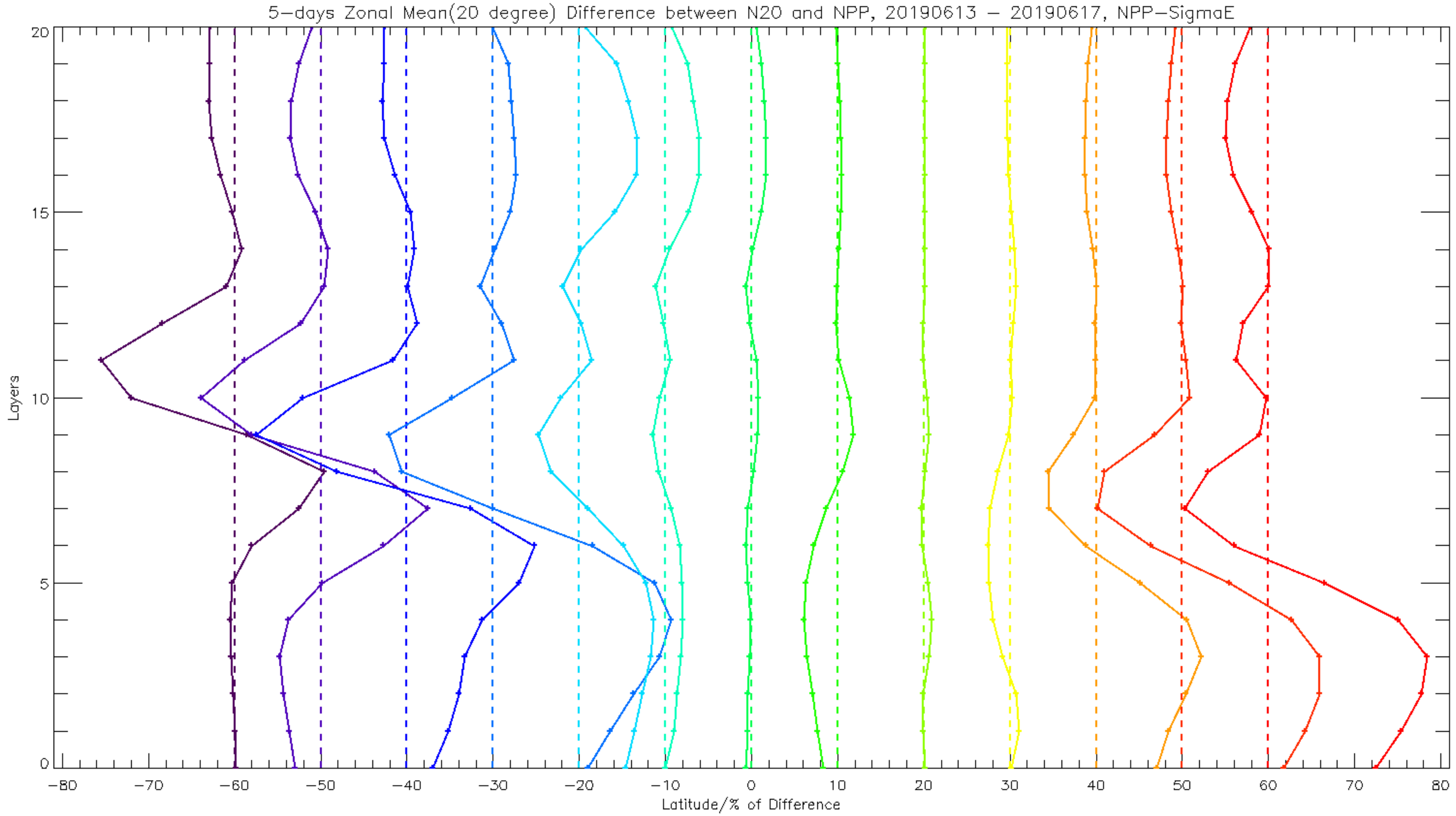


Initial Residual, OMPS N20(red) vs. OMPS NPP(black), Zonal Mean(20S−40S)
Error Bar = STDDEV
Residual
Channel, NM
4
2
0
−2
−4
250
260
270
280
290
300
310
320


Final Residual, OMPS N20(red) vs. OMPS NPP(black), Zonal Mean(20S–40S)
Error Bar = STDDEV
Residual
Channel, NM
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
250
260
270
280
290
300
310
320

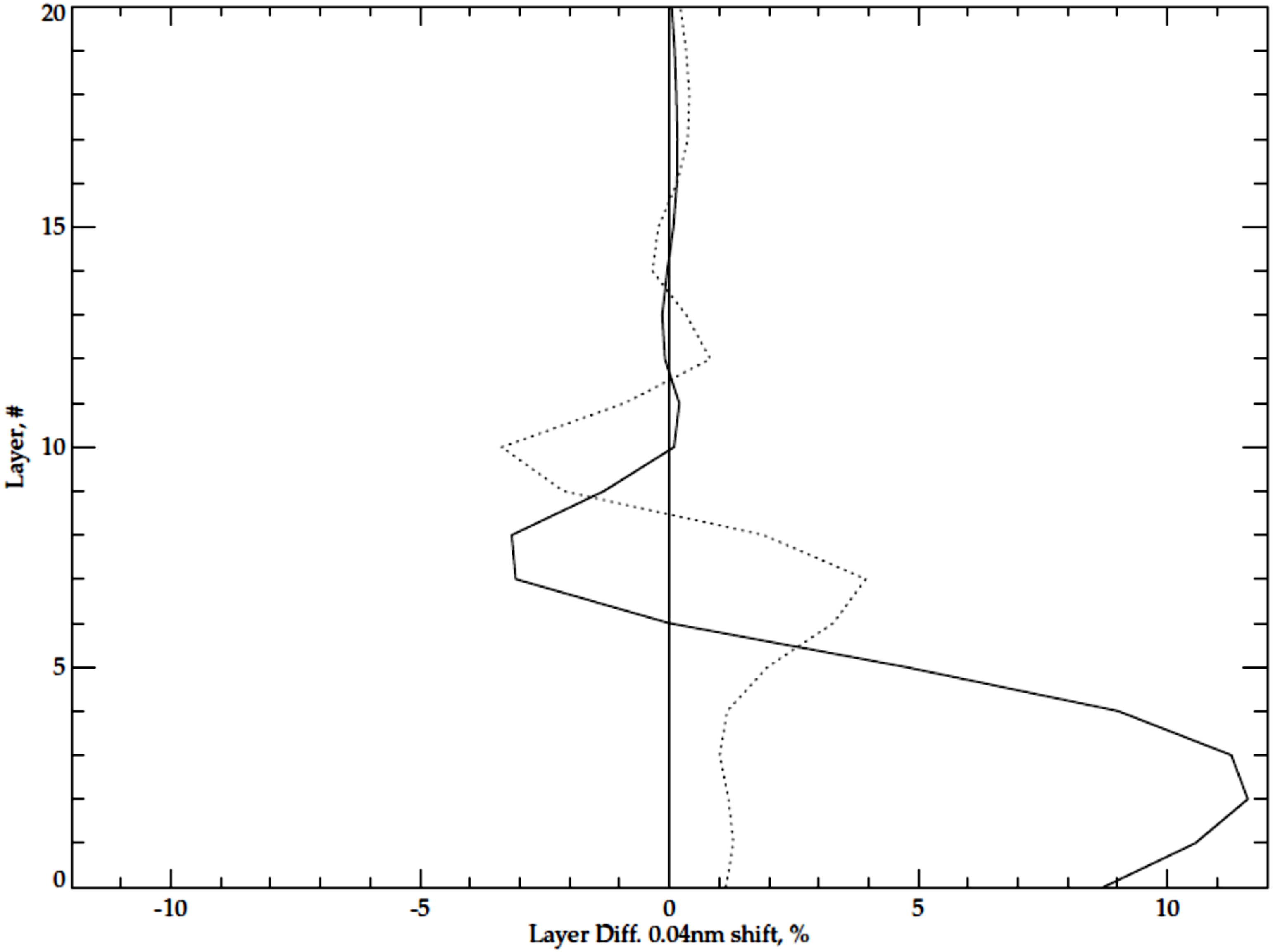


zone profile, OMPS N20(green) vs. OMPS NPP(black), Zonal Mean(20S–40
Red line = %–difference between OMPS N20 and NPP
Layers
Average Layers in DU

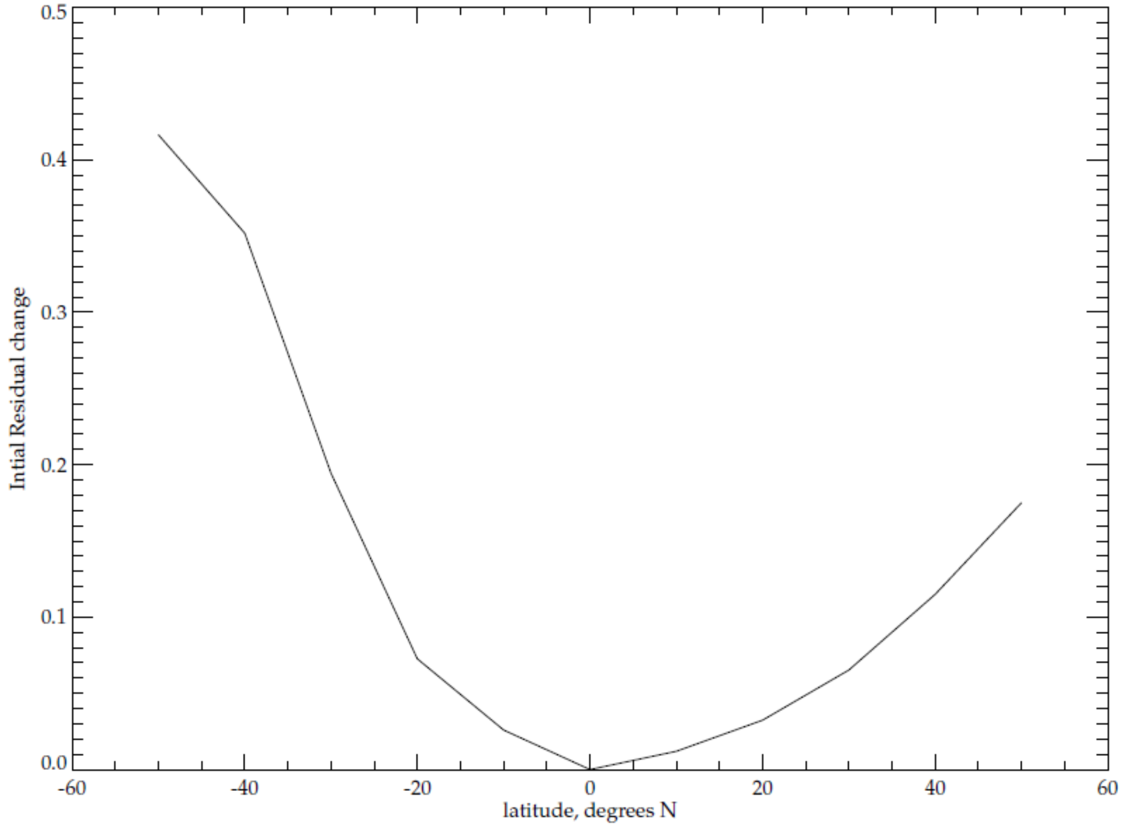


5–days Zonal Mean(20 degree) Difference between N20 and NPP, 20190613 – 20190617, NPP–SigmaE
Layers
20
15
10
5
0
–80
–70
–60
–50
–40
–30
–20
–10
0
10
20
30
40
50
60
70
80
Latitude/% of Difference

Sensitivity to 0.04-nm shifts for 302 nm channel [50N-E solid, 50S-E dotted]



Sensitivity to 0.04-nm shifts for 302 nm channel Initial Residuals compared to Equatorial change



BETA MATURITY FOR NOAA-20 OMPS

L. Flynn and NOAA-20 OMPS EDR and SDR Teams

March 15th, 2018

April 18th, 2018

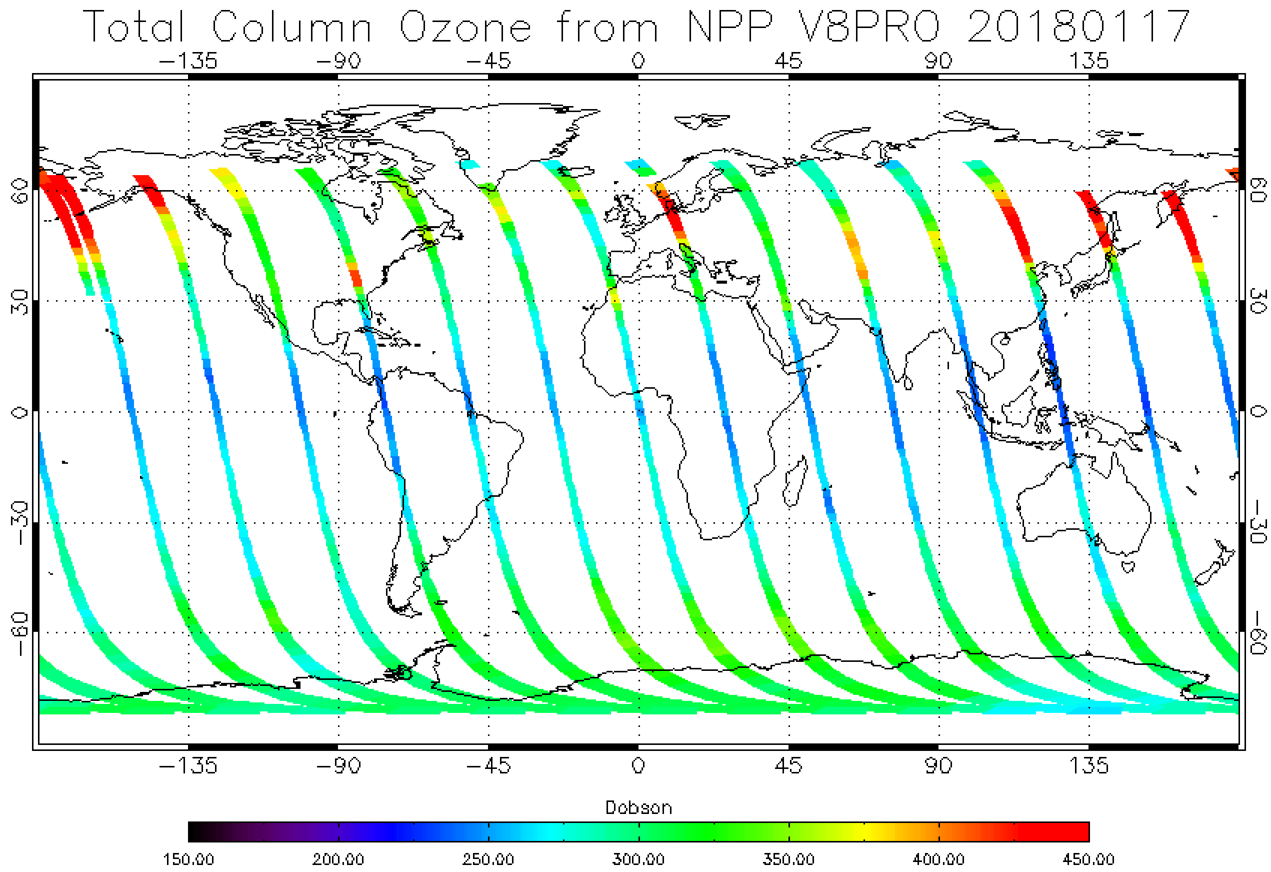
Summary of Findings for Ozone Profile EDR

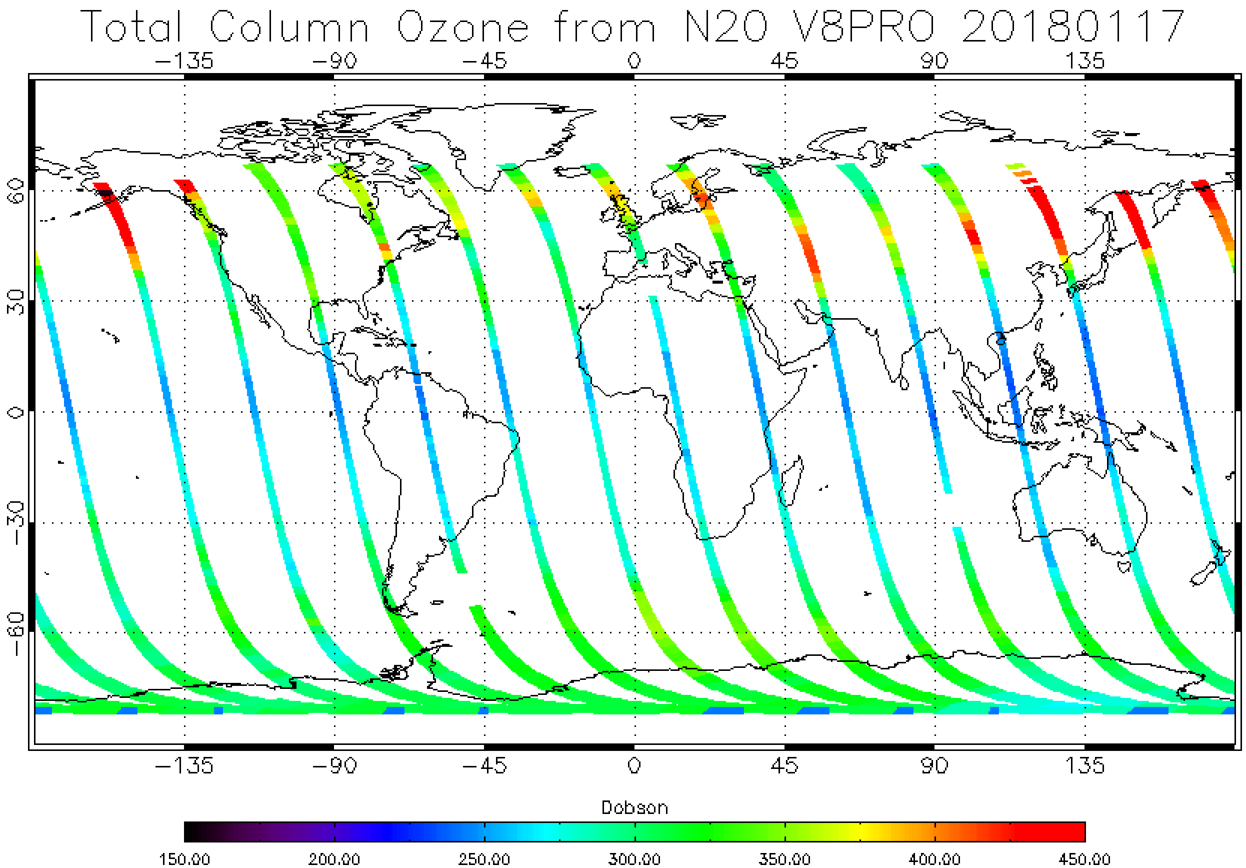
- NOAA-20 OMPS Nadir Profiler / V8Pro EDR*
  - EOF analysis of measurements shows good SNRs. Outliers are larger by linear factors in FOV size not square root factors. EDRs will be adversely affected by this noise.
  - EDRs show good results for this stage of maturity.
  - Output error for Profile Error Code 8 cases (Excessively large initial residual – Flag is correctly set). Code fix will be delivered to NDE with Provisional Table updates.
  - Code error in cross-track macropixel computation; fix expected at IDPS in July 2018.
  - New OMPS Nadir Profile sample table needed to match OMPS Nadir Mapper FOV.
  - Temporal aggregation of 15-scan NM RDRs to 5-scan RDRs causes offset between NM and NP. This was resolved with 15-scan SDR products in use since 3/30/2018.
  - Radiation in the SAA has a large effect on radiances for 50x50km^2 FOVs, some just outside of geographic flagged region.
  - Some cases of negative radiances are found in the auroral oval.
  - Dichroic effects on wavelength/bandpass and on calibration from 0.2-nm shift not yet accounted for in SDR calibration tables or EDR bandpass adjustments.
  - Possible overcorrection for stray light (not shown) leads to negative correlation between reflectivity and upper level ozone.

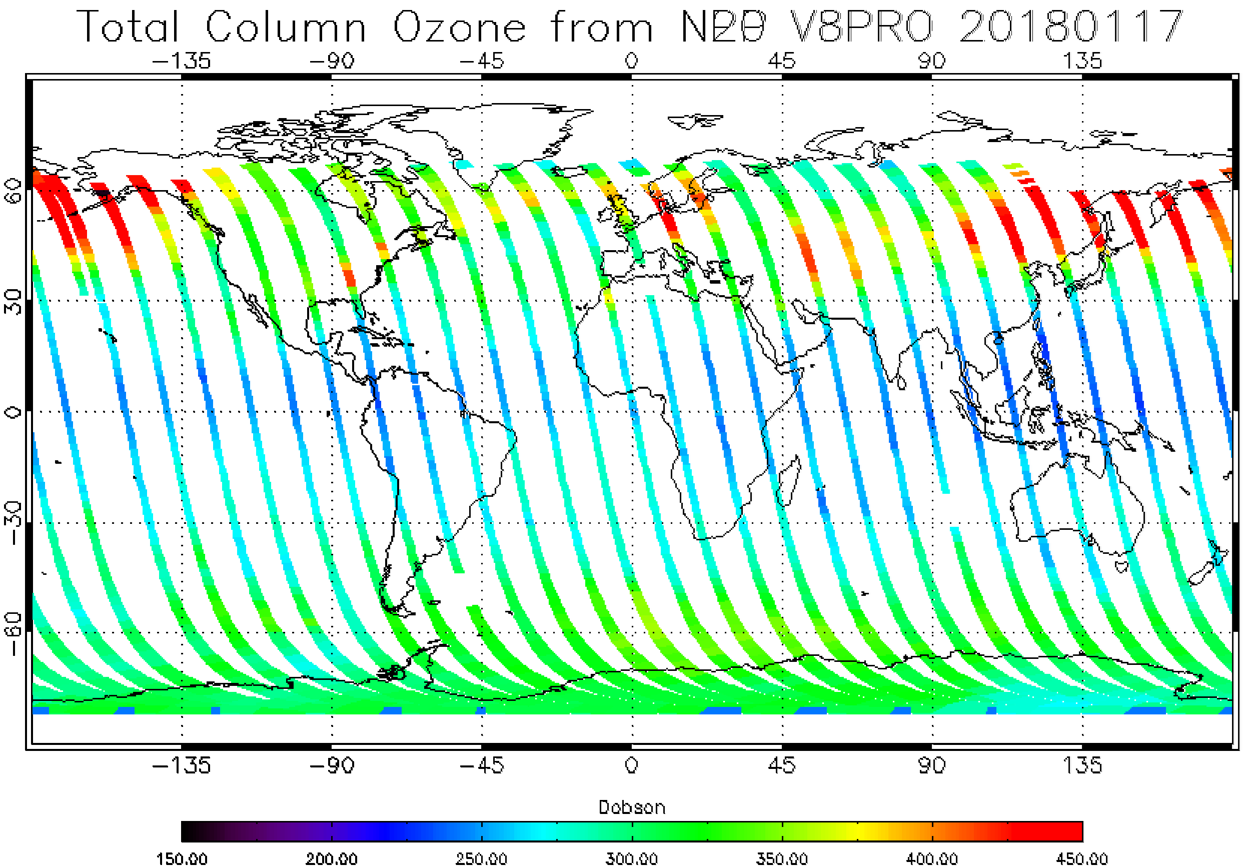
* Version 3 Revision 1 at NDE Operations and I&T

Provisional Delivery to NDE planned for May

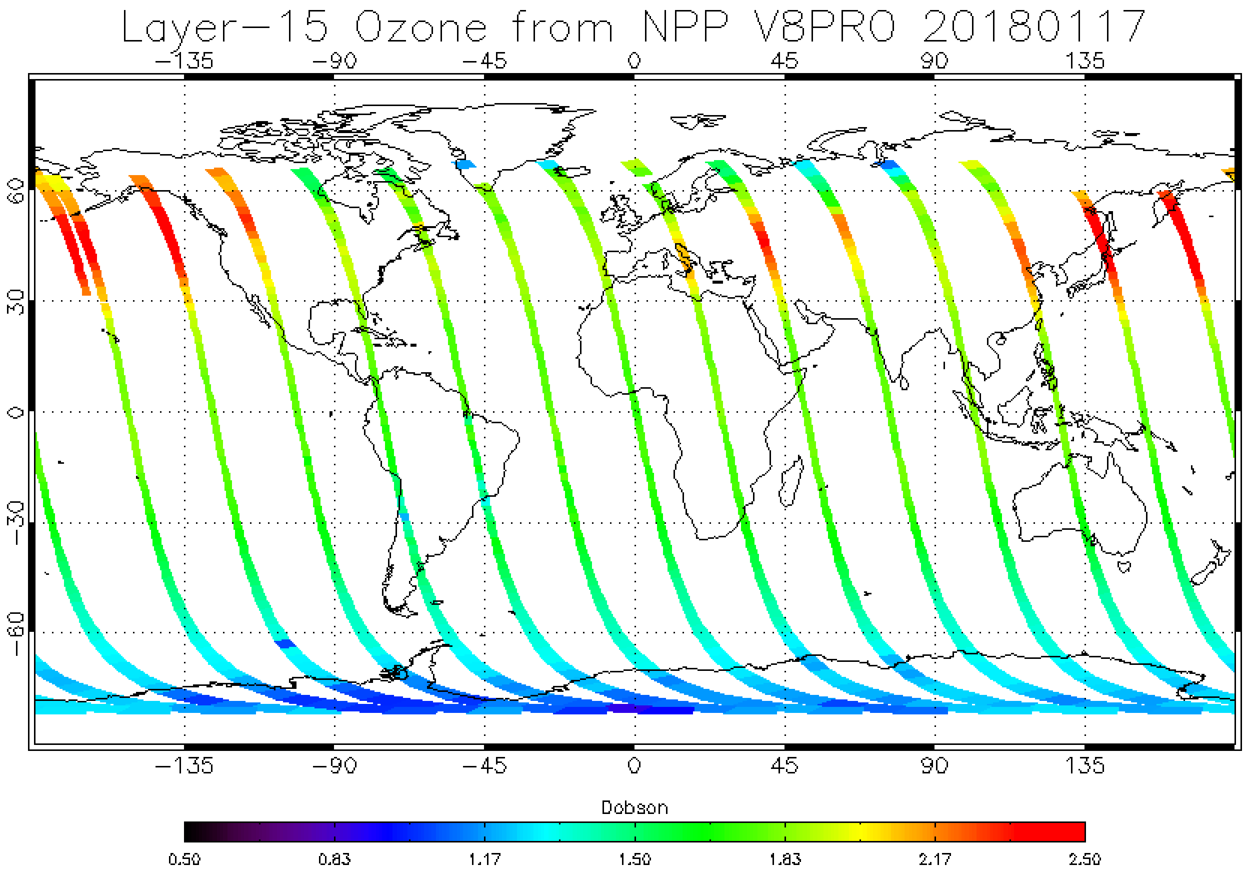
- Planned code, script and table changes at NDE
  - Given the range of SDR FOV sizes, we will provide dynamic SDR sizing adjustment for NM SDRs in codes, not control scripts. That is, the NDE operator will not need to know when the SDRs have switched to new sample tables and make manual adjustments to the scripts.
  - Improved handling of end of orbit, end of day, and duplicate granules
  - Fix for Profile Error Code 8 output EDR content for V8Pro.
  - Check FOV alignment accuracy for NM and NP within code by computing average latitude and longitude of contributing FOVs.
  - New adjustment tables for V8TOz and V8Pro
    - Requires access to SDRs with better sample tables
    - Requires access to SDRs with better stray light corrections
  - Test data processing to confirm LFSO2 is ready for smaller FOV V8TOz EDRs from NOAA-20 and improve 15-granule processing.

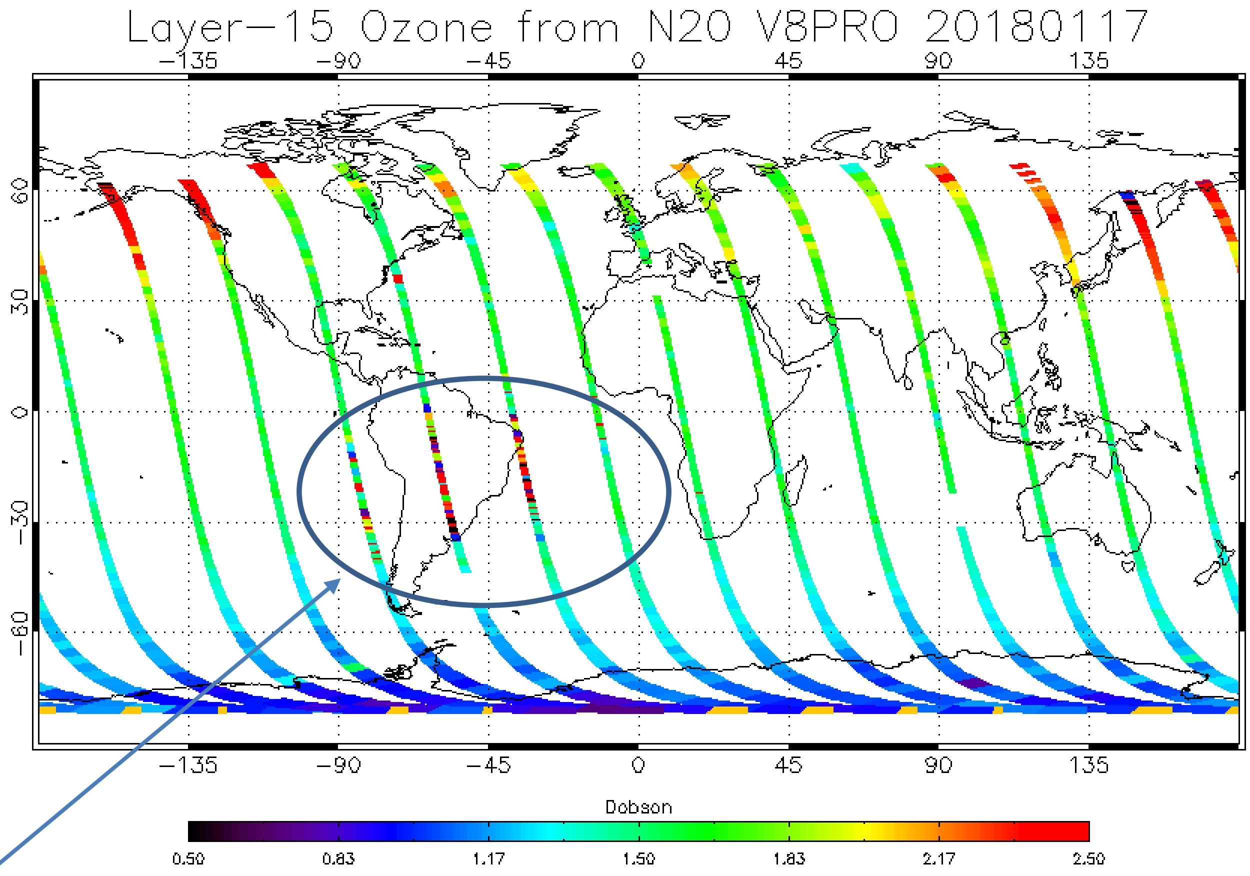

Total Column Ozone from NPP V8PRO 20180117
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
Dobson
150.00
200.00
250.00
300.00
350.00
400.00
450.00


Total Column Ozone from N20 V8PRO 20180117
-135 -90 -45 0 45 90 135
60 30 0 -30 -60
Dobson
150.00 200.00 250.00 300.00 350.00 400.00 450.00

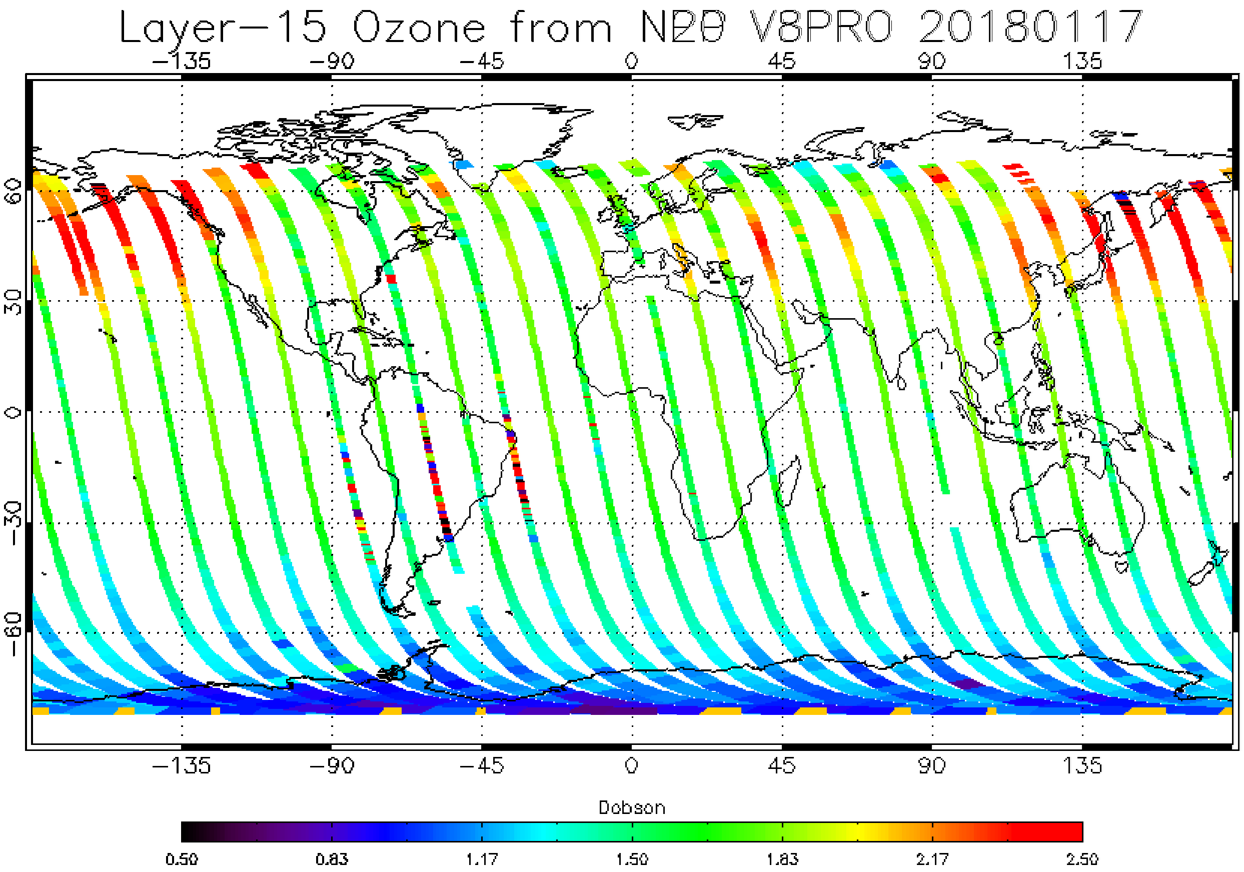


S-NPP and NOAA-20 OMPS Nadir Profile Total Column EDRs show good consiste


Layer−15 Ozone from NPP V8PRO 20180117
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
Dobson
0.50
0.83
1.17
1.50
1.83
2.17
2.50

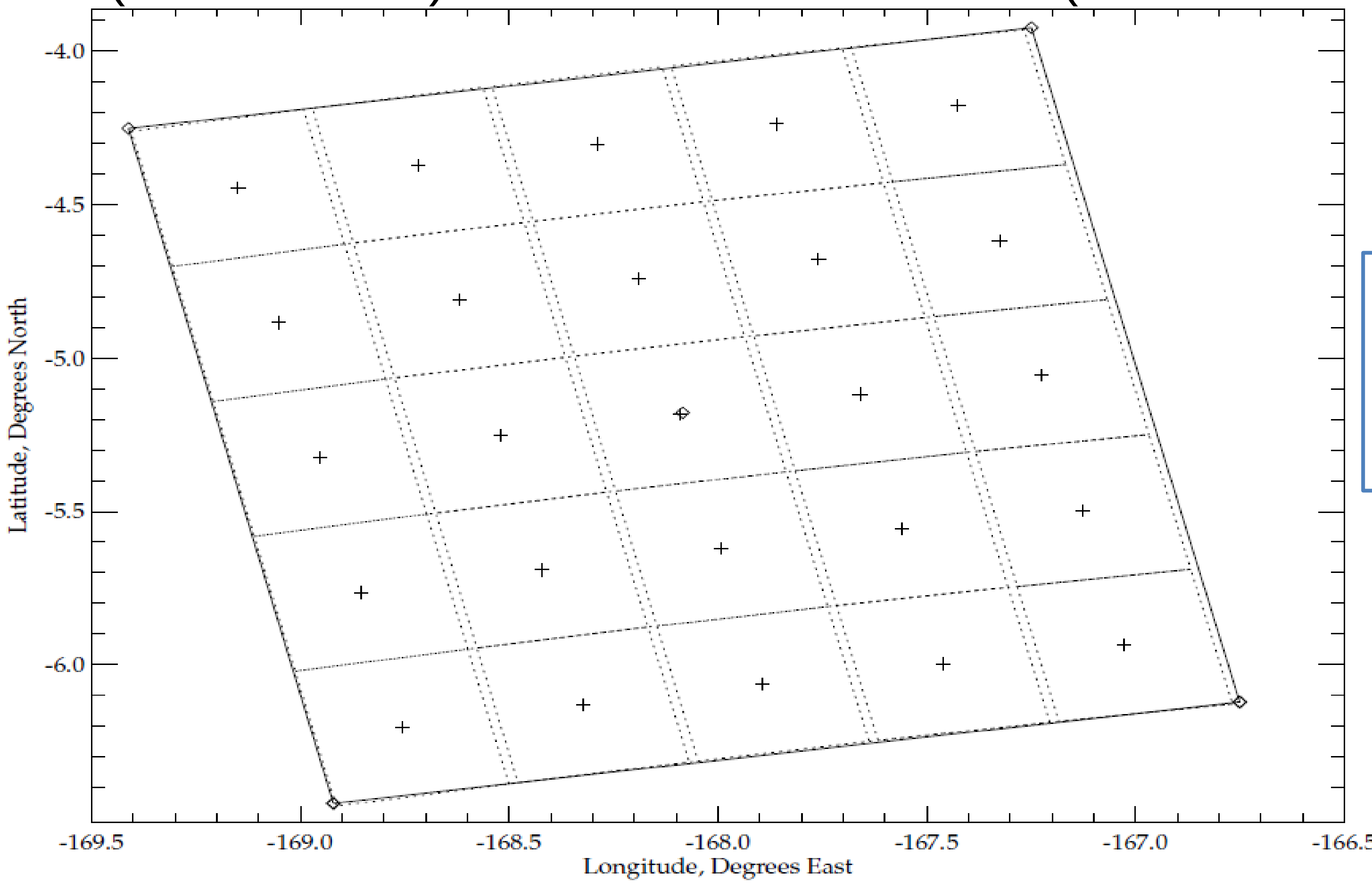


South Atlantic Anomaly



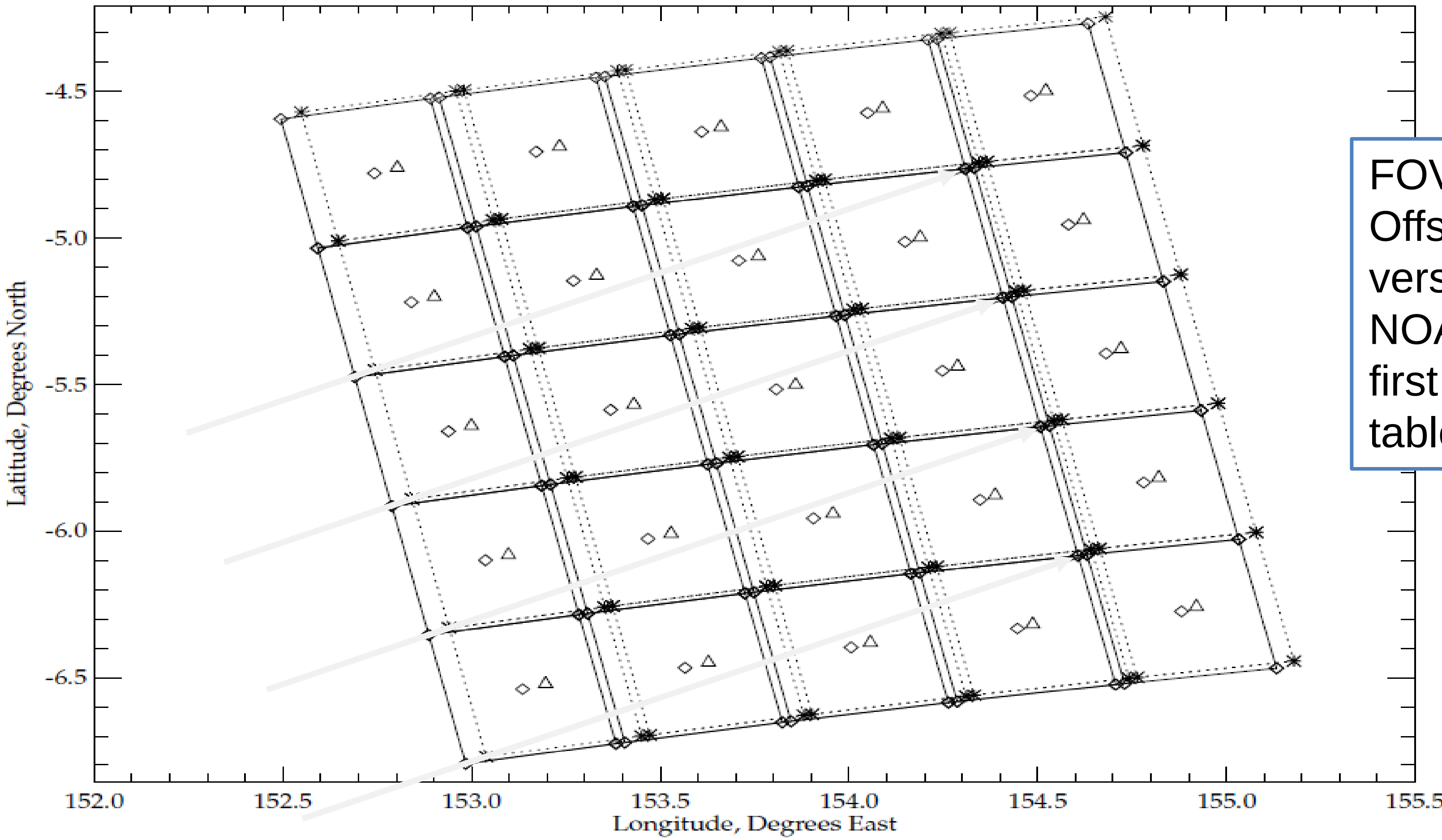
S-NPP and NOAA-20 OMPS Nadir Profile Layer Ozone EDRs show good consiste

Sample Matchup of FOVs for one Granule of S-NPP Nadir Mapper (Dotted and +) and S-NPP Nadir Profiler (Solid and <>)

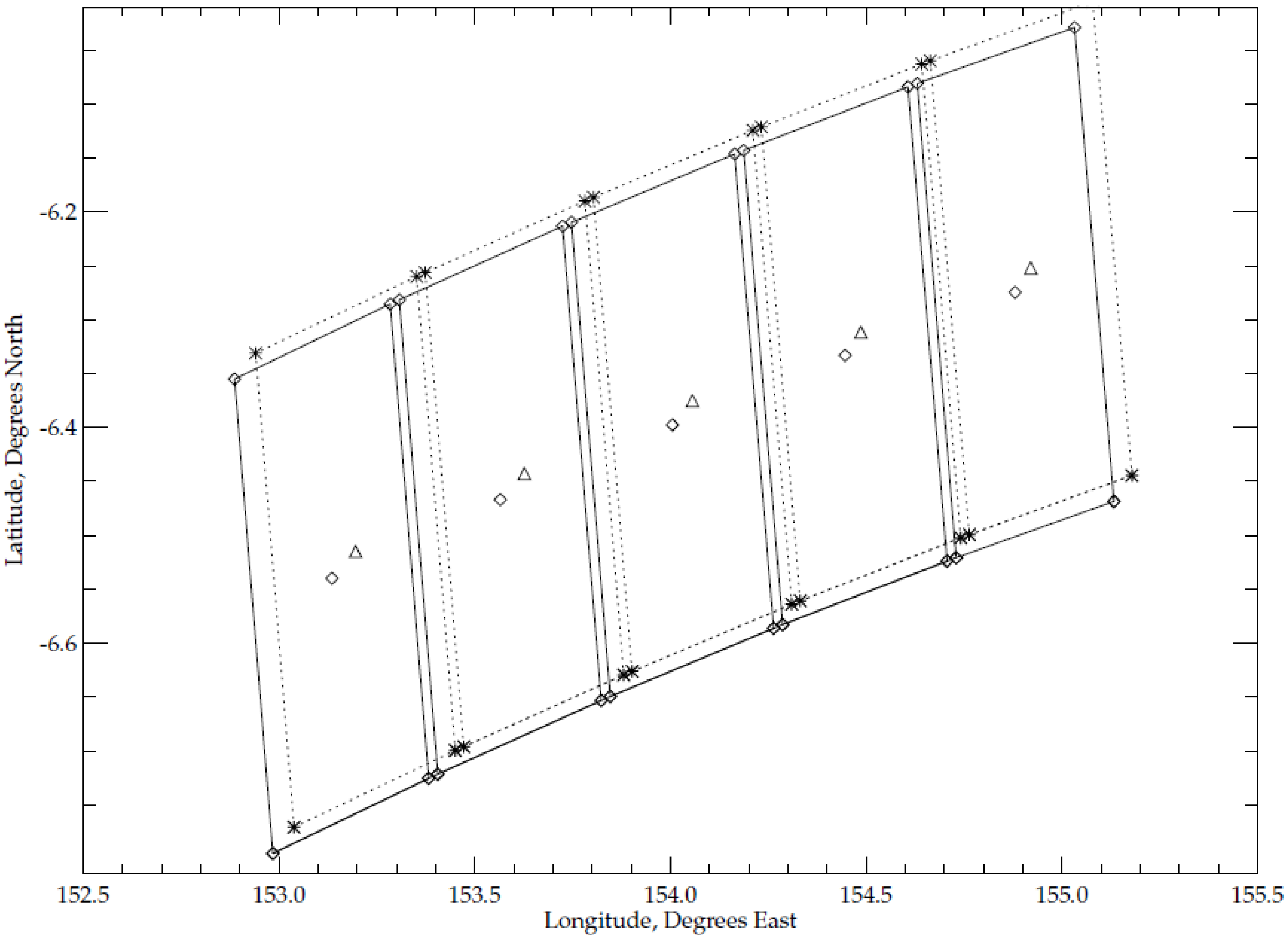


Boundaries match within one pixel width

Sample Matchup of FOVs for one Granule of NOAA-20 Nadir Mapper (Dotted & Δ) and NOAA-20 Nadir Profiler (Solid & <>)



FOV Match-Up Offsest for NM versus NP for NOAA-20 with first sample tables.



FOV Match-Up:
Same as Slide 14 but just for the lowest row / first scan.
Note the along-track offsets – top and bottom shifts of ~2 km.

Summary & Conclusions

- The NOAA-20 OMPS Ozone EDR and BUFR products are ready for users to examine. They have proper formatting and reasonable values for content.
- Deficiencies in the OMPS SDRs are known, and the SDR Team has paths forward to improve the products.
- Minor code and script changes will be provided to NDE for the V8Pro, V8TOz and LFSO2 codes in a May 2018 delivery.
- Final adjustment tables for the EDR products will be developed by using off-line STAR SDR processing.
- Product quality will improve as SDR and EDR Team adjustments and corrections enter the IDPS and NDE processing systems.

IMPROVEMENTS, CORRECTIONS AND REFINEMENTS FOR THE NEXT OMPS V8PRO BUILD FOR NDE

L. Flynn, Z. Zhang, E. Beach, T. Beck, J. Niu

- The updated scripts and codes:

```
./bin/run_v8pro_nde.sh    (for NDE environment)
./bin/run_v8pro_star.sh   (for STAR environment)

./src/constants.f90
./src/control.f90
./src/data_ingest.f90
./src/init_retrieval.f90
./src/netcdf_util.f90
./src/O3P_main.f90
./src/profile.f90
./src/profile_datamod.f90
./src/scanin.f90
./src/start.f90
./src/total.f90
```

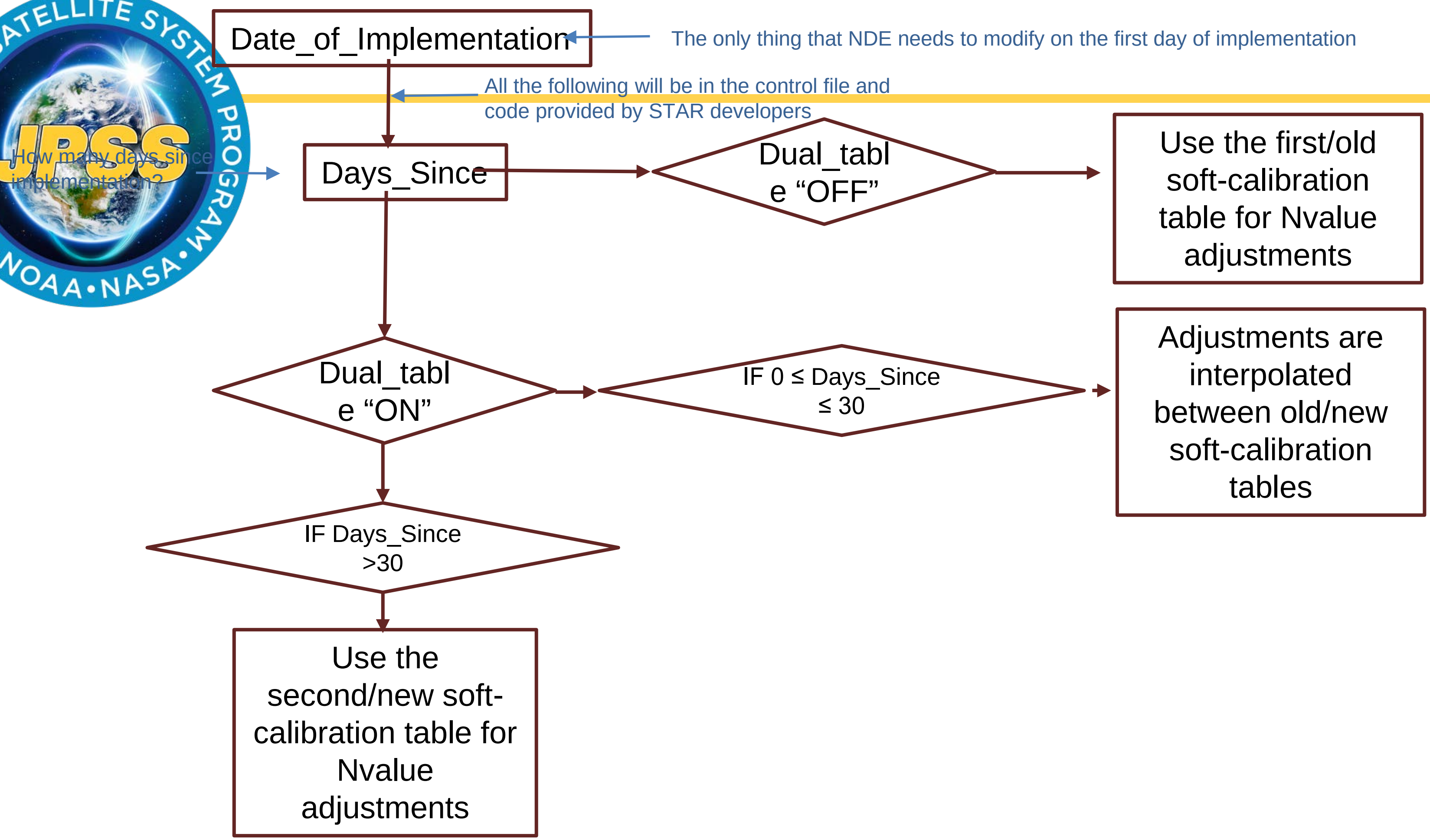
Outline

- A. Dual Adjustment Tables
  - Provide Old (Current) and New (Updated) soft calibration tables with the option to interpolate between them to smooth the transition. File names will have creation dates.
- B. Metadata improvements.
  - Additional fields are added to metadata to be consistent with NDE requirements and to provide better information. These include the NDE production site, NDE production environment, and the adjustment table's file name.
- C. Area-Weighted FOV Averages
  - When the NOAA-20 OMPS NM goes to [10,10,10,10, 5, 10, 5, 10, 10, 10, 10] pixel aggregation, we will want to have area-weighted values computed in the glueware. This refinement provides the code to calculate and use the relative sizes of the FOVs.
- D. Remove the use of 340 nm channel for reflectivity.
  - Code updates to switch from 340 nm channel to 331 nm channel for some reflectivity calculations for consistency with the NASA V8Pro implementation.
- E. Code Fixes
  - Averaging Kernels: Change OMPS V8Pro product configuration for the averaging kernels to agree with the SBUV/2 relative response one.
  - Mixing ratio inconsistency in amount and pressure order.
  - Terrain Pressure maximum and minimum extended to include Dead Sea and Mt. Everest.
  - Descending orbit data are not processed – fix by changing corner order in Glueware.
- F. Change to handle OMPS NM SDR sizes up to 30 scans x 140 cross-track FOVs per granule.
- G. Outlier Detection Filter and Information Concentration (F&IC)
  - Implement a combination of median filter and 10- to 12-wavelength polynomial fits of the radiance / irradiance ratios for the shorter ozone profile channels to reduce measurement noise, remove outliers and identify PMCs.

A. Dual Adjustment Tables (1/3)

- The OMPS NP sensors have small throughput degradation over time but even so need periodic adjustments to the channels for radiances used in the V8Pro retrieval algorithm. The current code reads in a single set of adjustments so when a table is changed there is a discontinuity in the product. Such jumps create problems for users assimilating our ozone products as they appear in the observed minus forecast statistics. For SBUV/2 V8Pro, changes in the adjustments are put in over a 30-day window with 1/30 more of the jump effected each day.
- We are refining the V8Pro code for OMPS to accept dual adjustment tables with the old and new values present and to interpolate between the two over an input-controlled time period to allow similar performance for OMPS V8Pro EDRs. The code will linearly interpolate between the two during a configurable (by control scripts) transition period on the order of 30 (TBR) days.

A. Dual-table processing flow chart (2/3)



A. Dual-table Control File Changes (3/3)

Below is the section in the PCF file that NDE needs to modify on the first day of implementation

```
#######################################################
##########    For NDE changes   ########################
#######################################################
##---First time when implementing to a new site/environment, we need to update---##
    #  p_environment="DEV/TST/OPS"
    #  p_site="STAR/NDE"
      p_environment="DEV"
      p_site="STAR"
    # DateToImplement="Jan/Feb/Mar/Apr/May/Jun/Jul/Aug/Sep/Oct/Nev/Dec dd(01/02/...31)
yyyy"
      DateToImplement="Mar 21 2019"
##---End of update for the first time of implementation---##
#######################################################
##########    End of For NDE changes   #################
#######################################################
```

B. Metadata in the next OMPS V8PRO delivery, 1/2

V8PRO-EDR_v3r3_npp_s201512280110098_e201512280110472_c201903281426370.nc (0)
    Group size = 67
    Number of attributes = 41
        Convention = CF-1.5
        Metadata_Conventions = CF-1.5, Unidata Datasset Discovery v1.0
        Metadata_Link = V8PRO-EDR_v3r3_npp_s201512280110098_e201512280110472_c201903281426370.nc
        _nc3_strict = 1
        ascend_descend_data_flag = 0
        creator_name = DOC/NOAA/NESDIS/STAR > OZONE Algorithm Team, Center for Satellite Applications and Research, NESDIS, NOAA, U.S. Department of Commerce
        date_created = 2019-03-28T14:26:37Z
        day_night_data_flag = 1
        end_orbit_number = 21588
        geospatial_bounds = POLYGON((-173.53 -21.63, -171.18 -21.28, -171.74 -19.09, -174.05 -19.44, -173.53 -21.63))
        geospatial_first_scanline_first_fov_lat = -21.28
        geospatial_first_scanline_first_fov_lon = -171.18
        geospatial_first_scanline_last_fov_lat = -21.63
        geospatial_first_scanline_last_fov_lon = -173.53
        geospatial_last_scanline_first_fov_lat = -19.09
        geospatial_last_scanline_first_fov_lon = -171.74
        geospatial_last_scanline_last_fov_lat = -19.44
        geospatial_last_scanline_last_fov_lon = -174.05
        geospatial_lat_units = degrees_north
        geospatial_lon_units = degrees_east
        history = Created by V8PRO version 1.0, Release 0.0
        id = esz37f5s-djh8-4619-8274-3zd8559knb3t
        institution = NOAA/NESDIS
        instrument_name = OMPS
        naming_authority = gov.noaa.nesdis.star
        platform_name = NPP
        processing_level = EDR

B. Metadata in the next OMPS V8PRO delivery, 2/2

*New content

```
#   production_environment="DEV/TST/OPS"
#   production_site="STAR/NDE"
```

production_environment = DEV
production_site = STAR
project = NOAA V8PRO
publisher_email = espcoperations@noaa.gov
publisher_url = http://www.star.nesdis.noaa.gov
source = NP Granule --
>>../input_dat/SOMPS/SOMPS_npp_d20151228_t0110098_e0110472_b21588_c20151228083103578783_noaa_ops.h5../input_dat/GONPO/GONPO_npp_d20151228_t0110098_e0110472_b21588_c20151228080021376593_noaa_ops.h5<< First NM Granule --
>>../input_dat/SOMTC/SOMTC_npp_d20151228_t0110098_e0110472_b21588_c20151228080952714003_noaa_ops.h5../input_dat/GOTCO/GOTCO_npp_d20151228_t0110098_e0110472_b21588_c20151228080015994702_noaa_ops.h5<< Second NM Granule --
>>../input_dat/SOMTC/SOMTC_npp_d20151228_t0110472_e0111246_b21588_c20151228080952714003_noaa_ops.h5../input_dat/GOTCO/GOTCO_npp_d20151228_t0110472_e0111246_b21588_c20151228080015994702_noaa_ops.h5
standard_name_vocabulary = CF Standard Name Table (version 1, 24 Jan. 2015)
start_orbit_number = 21588
starting_and_ending_orbit_node = AA
status_info = Implemented at STAR/DEV on Mar 21 2019 with dual_table ON, and has run 7 days using soft_cali_table ../data/band_centers20190318.txt and ../data/band_centers20180518.txt
summary = V8PRO retrieved ozone profile, total column amount of ozone, and aerosol index
time_coverage_end = 2015-12-28T01:10:47Z
time_coverage_start = 2015-12-28T01:10:09Z
title = V8PRO L2

C. Area-Weight

Code changes to implement
area weighting for glueware.

We could compute average latitude and longitude to check on how well NM FOVs match NP FOVs or we could use wpp.

Changes for the ascending/descending also are present in this subroutine. If descending conditions are present, the corner order is switched to [3,4,1,2] .

```
wpp=0.0
DO i=1, nxtrc ! search all points within NP nadir FOV
    DO j=1, nline+nline
        x_lo = (nmlat(i,j)-nplat(1))*(nplon(2)-nplon(1))/&
               (nplat(2)-nplat(1)) + nplon(1)
        x_hi = (nmlat(i,j)-nplat(3))*(nplon(4)-nplon(3))/&
               (nplat(4)-nplat(3)) + nplon(3)
        y_lo = (nmlon(i,j)-nplon(1))*(nplat(4)-nplat(1))/&
               (nplon(4)-nplon(1)) + nplat(1)
        y_hi = (nmlon(i,j)-nplon(2))*(nplat(3)-nplat(2))/&
               (nplon(3)-nplon(2)) + nplat(2)
        if ((nmlon(i,j) .ge. x_lo) .and. (nmlon(i,j) .le. x_hi) .and. &
            (nmlat(i,j) .ge. y_lo) .and. (nmlat(i,j) .le. y_hi)) then
           if (isnan(nmwave_m(30)) .or. nmwave_m(30) .lt. 0. .or. &
               isnan(nmwave(30,i)) .or. nmwave(30,i) .lt. 0. .or. &
               isnan(nmrad_m(30)) .or. nmrad_m(30) .lt.  0. .or. &
               isnan(nmrad(30,i,j)) .or. nmrad(30,i,j) .lt. 0. .or. &
               isnan(nmirad_m(30)) .or. nmirad_m(30) .lt. 0. .or. &
               isnan(nmirad(30,i)) .or. nmirad(30,i) .lt. 0. ) then
               WRITE(6,*) 'Warning pixel found at searching region'
           ELSE
               warea2=areadeg2(nmlonc(1:4,i,j),nmlatc(1:4,i,j))
               ipp=ipp+1.
               wpp=wpp+warea2
               nmwave_m(1:mwave)=nmwave_m(1:mwave) + nmwave(1:mwave,i)*warea2
               nmrad_m(1:mwave)=nmrad_m(1:mwave) + nmrad(1:mwave,i,j) *warea2
               nmirad_m(1:mwave)=nmirad_m(1:mwave) + nmirad(1:mwave,i) *warea2
           endif
         endif
     enddo
 enddo
 nmwave_m(1:mwave)=nmwave_m(1:mwave)/wpp
 nmrad_m(1:mwave)=nmrad_m(1:mwave)/wpp
 nmirad_m(1:mwave)=nmirad_m(1:mwave)/wpp
! Do not divide by ipp. Check on value of ipp?
```

C. Area-Weight

```
; IDL Code to compute area in degrees latitude squared from four corner points.
function areadeg2,lonc,latc
; lonc(4), latc(4)
  latw1=abs(latc(0)-latc(1))
  lath1=abs(latc(1)-latc(2))
  latw2=abs(latc(2)-latc(3))
  lath2=abs(latc(3)-latc(0))
  coslatw1=cos((latc(0)+latc(1))*!pi/360.0)
  coslath1=cos((latc(1)+latc(2))*!pi/360.0)
  coslatw2=cos((latc(2)+latc(3))*!pi/360.0)
  coslath2=cos((latc(3)+latc(0))*!pi/360.0)
  lonw1=lonc(0)-lonc(1)
if (lonc(0)*lonc(1) lt 0 and (lonc(0) gt 100 or lonc(1) gt 100)) then $
      lonw1=360.-abs(lonc(0))-abs(lonc(1))
  lonw1=abs(lonw1)*coslatw1
  lonh1=lonc(1)-lonc(2)
if (lonc(1)*lonc(2) lt 0 and (lonc(1) gt 100 or lonc(2) gt 100)) then $
      lonh1=360.-abs(lonc(1))-abs(lonc(2))
  lonh1=abs(lonh1)*coslath1
  lonw2=lonc(2)-lonc(3)
if (lonc(2)*lonc(3) lt 0 and (lonc(2) gt 100 or lonc(3) gt 100)) then $
      lonw2=360.-abs(lonc(2))-abs(lonc(3))
  lonw2=abs(lonw2)*coslatw2
  lonh2=lonc(3)-lonc(0)
if (lonc(3)*lonc(0) lt 0 and (lonc(3) gt 100 or lonc(0) gt 100)) then $
      lonh2=360.-abs(lonc(3))-abs(lonc(0))
  lonh2=abs(lonh2)*coslath2
  width=(sqrt(lonw1^2+latw1^2)+sqrt(lonw2^2+latw2^2))/2.
  height=(sqrt(lonh1^2+lath1^2)+sqrt(lonh2^2+lath2^2))/2.
  areadeg=width*height
return,areadeg
end
```

D. Switch back to 331 nm channel for reflectivity

NASA V8Pro does not use the 340 nm channel for reflectivity calculations. We will change the code to match their formulation. This will also be consistent with the earlier SBUV/2 record.

E. Code Fixes (1/4)

– Consistent Averaging Kernels for EDR and BUFR products

The subroutine convert20 in the SBUV/2 has an added comment and code.

"Transform the 20-layer averaging kernel form absolute form into relative (fractional) form.“

```
c
c     Transform AK into fractional form
c
      do k = 1,20
        do l = 1,20
          avkernp(k,l) = avkernp(k,l)*qap(l)/qap(k)
        end do
      end do
c
```

where qap(21) was calculated from qa(81) as:

```
      do k = 1,20
        i1 = (k-1)*4 + 1
        qap(k) = qa(i1) + qa(i1+1) + qa(i1+2) + qa(i1+3)
      end do
      qap(21) = qa(81)
```

There was no such transformation in the current OMPS V8PRO.

E. Code Fixes (2-4/4)

- Mixing ratio inconsistency in amount and pressure order.
  - PPMV Amounts are given top to bottom; hPa pressure is given bottom to top.
  - We will give the pressure top to bottom to be consistent. This will also correct the BUFR products as they use these values directly from the EDR.
- Terrain Pressure maximum and minimum extended.
  - Limits did not include some high pressure and Dead Sea Cases, and low pressure over regions over the Himalayas. New limits will give some margin on the realistic range of pressures
- Descending orbit data are not processed
  - The Glueware will be adjusted to correctly matchup OMPS NM and NP FOVs for descending orbit cases.

F. Change to handle OMPS NM SDR size 30x140 FOVs per granule

Change maximum array size of input to allow 30x140 OMPS MN SDR.

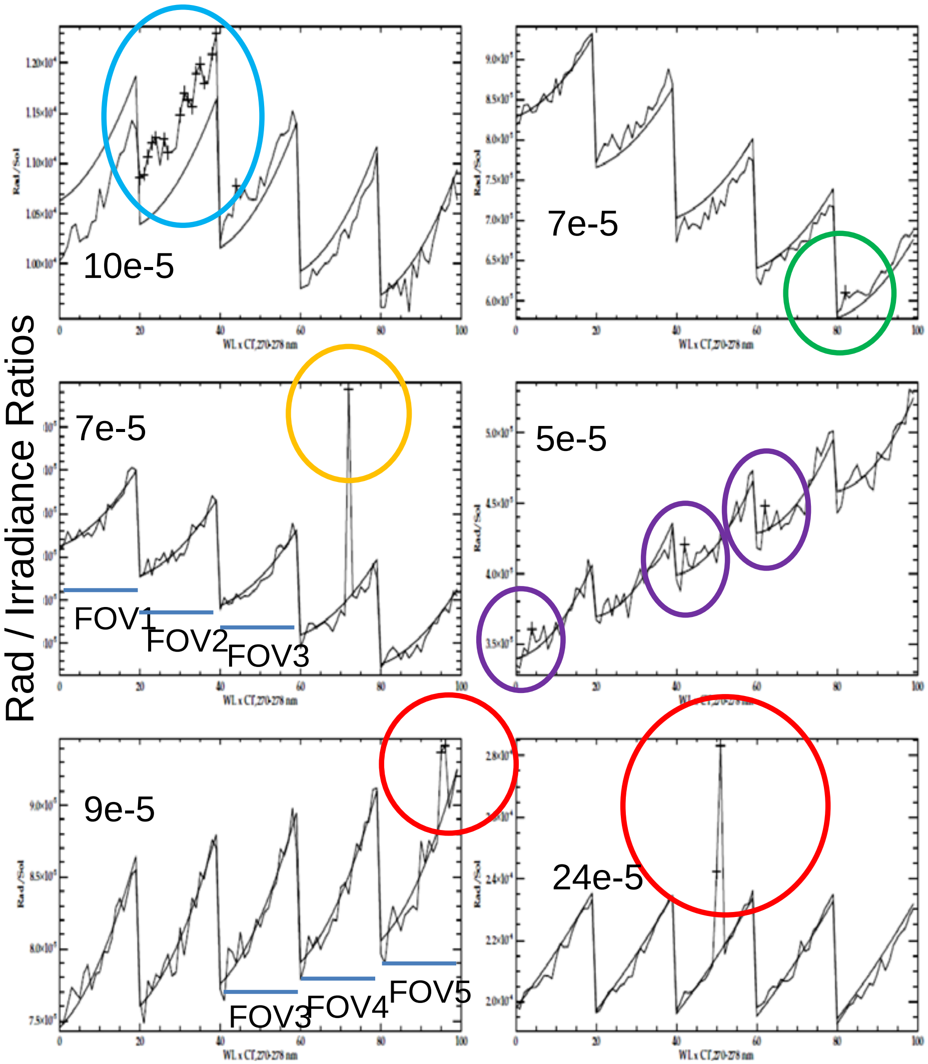
Check input nscan and nifov for OMPS NM SDR.

No change to output as NM data are aggregated to match OMPS NP FOVs. There will simply be a change to the number of scans and cross-track FOVs found and averaged by the glueware. We already loop over the nscan and nifov range to do this.

G. Outlier Detection Filter and Information Concentration

- The smaller fields of view (FOV) for NOAA-20 OMPS NP have greater sensitivity to noise and outliers. We had expected that this could be handled by increasing the measurement noise in the Optimal Estimation retrieval and included those changes in our last code update. The outliers do not scale like Gaussian noise and we need a more refined approach to handle the effects of charged particle hits. While investigating approaches to Filter the data & Concentrate Information (F&IC) at the V8PRo wavelength channels, we found that there were significant impacts on the radiances when Polar Mesospheric Clouds (PMCS) are present. The increased sensitivity of the smaller FOV data to variations in PMCs provides an opportunity to identity these as a part of the F&IC process. If the filtering process identifies too many bad values (e.g., within the SAA or in the high latitude Summer Hemisphere), then we will continue the retrieval but flag the data. The process uses a median filter followed by low degree polynomial fits in wavelength (about the target channels) and cross track (for each scan). The code will also detect the presence of PMCs. Spectra will be flagged if the number of outliers exceed a limit in any of the key spectral intervals. We will use radiance based limits instead of percent to deal with the changing signal levels. Parameters for the fit model and thresholds will be provided (read in) as part of existing tables or control files.

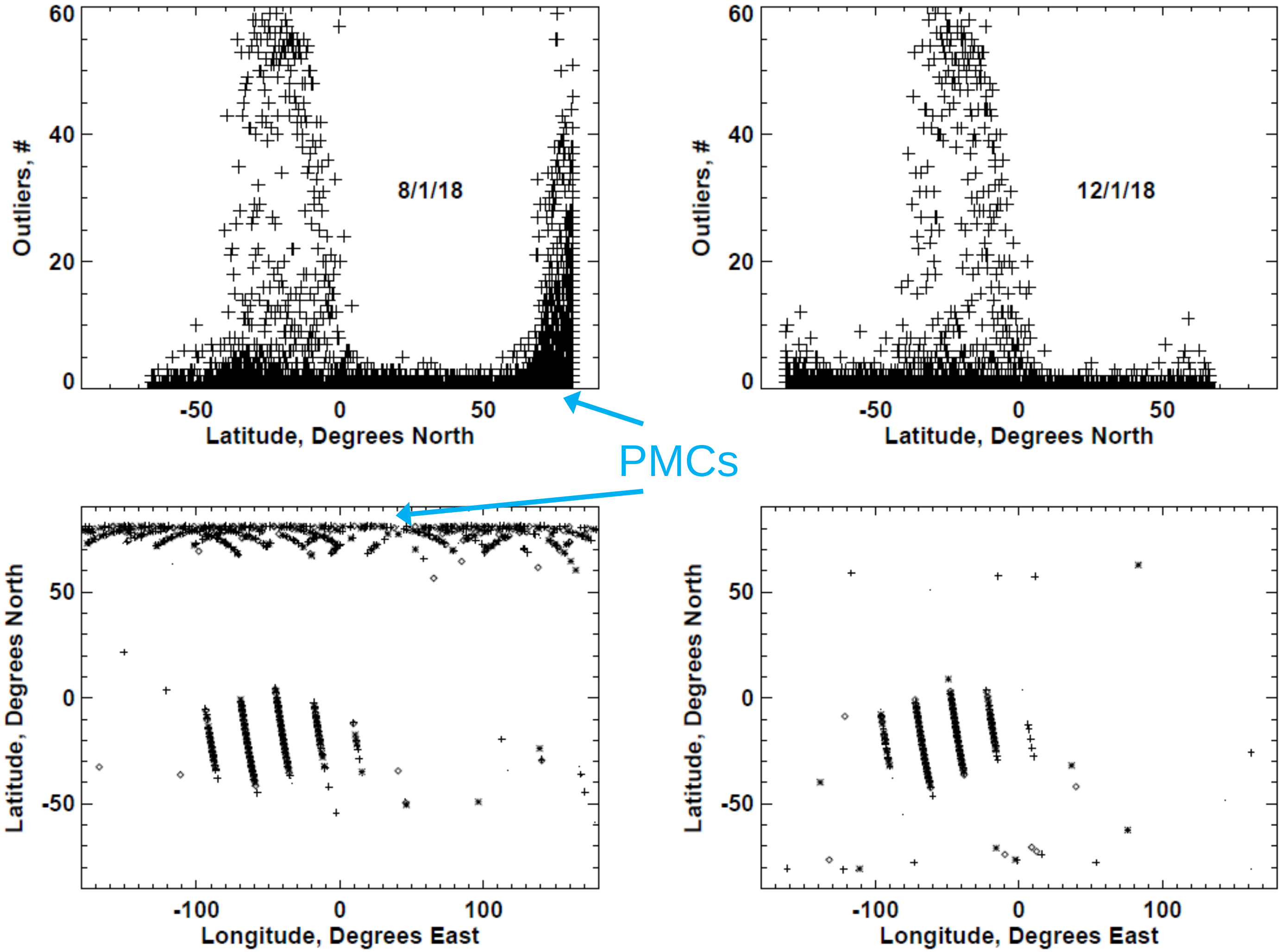
G. SPECTRAL AND SPATIAL FILTERING & INFORMATION CONCENTRATION RESULTS FOR NOAA-20 OMPS NP



NOAA-20 OMPS NP makes measurements of spectra for five cross track FOV for each scan; there are opportunities for filtering and information concentration making use of additional channels. A simple model was developed. Polynomial fits of radiance / irradiance ratios for channels in wavelength intervals centered at the V8Pro wavelengths are combined with a single linear function in the cross-track dimension fit by multiple regression. The fit is computed iteratively with outliers beyond a set threshold removed each time. The charged particle effects are usually positive. The final fit value at a selected wavelength can be used in the retrieval algorithm.

A sample set of results for six scans for August 1, 2018 is shown to the left. 20-wavelength (8-nm) intervals were centered at 274 nm with a quadratic polynomial for the spectral fit pattern and a linear function for the spatial cross track fit pattern. The smooth curves show the fits for the five cross-track wavelength intervals for each of the 20-wavelength intervals. The jagged lines are the measurement radiance / irradiance ratios.

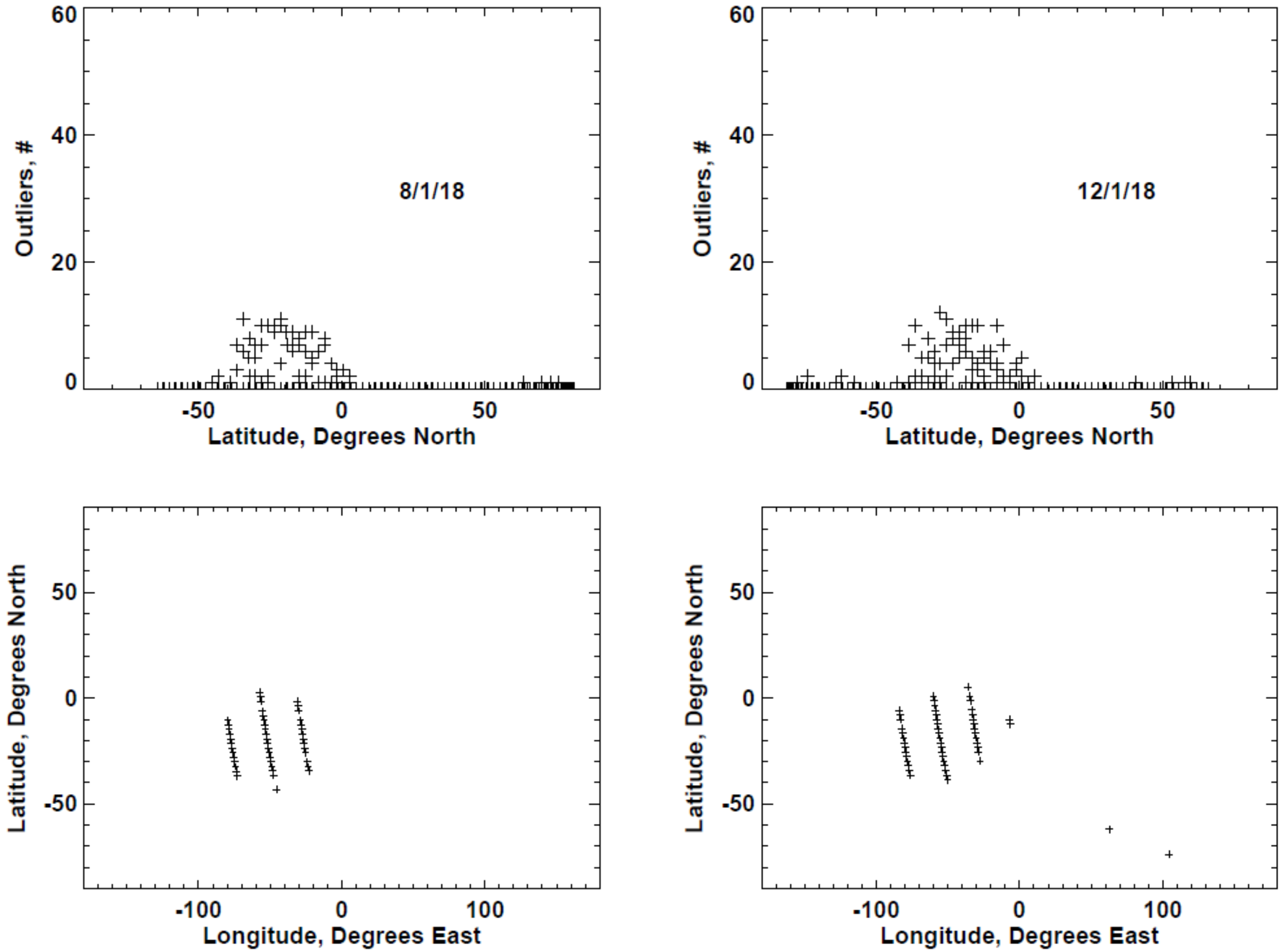
The threshold for the iterative point replacement was set at 4%. The majority of the fits do not have any values exceeding this limit. That is, no points are removed in the fitting process. The orange circle shows the next most likely case, where a single measurement has been affected by a charged particle hit on the CCD array. A + sign is used to indicate the offending value. The red circles show cases where two measurements exceed the residual threshold. The outliers for these two cases are both adjacent spectrally. The purple circles show a case where three values all for the same spectral row were identified as outliers. The orange and red cases occurred in the SAA. The blue circle shows a case at high latitude in the summer hemisphere where Polar Mesospheric Clouds (PMCs) are present in some of the FOVs and disrupt the cross-track pattern. Studies of SBUV/2 measurements have been used to create a climatology of PMCs [1]. The green circle shows a marginal case which may be due to PMCs, or may be caused by a charged particle hit in the auroral oval or may simply be a noisy measurement effect.



Number and location (for scans with five or more replaced values) of outliers for two days of NOAA-20 OMPS NP SDR data. Twelve wavelength intervals around 273 nm were used and each five cross-track FOV scan was fit with a linear regression using a quadratic model in wavelength and a linear model in cross-track FOV number.

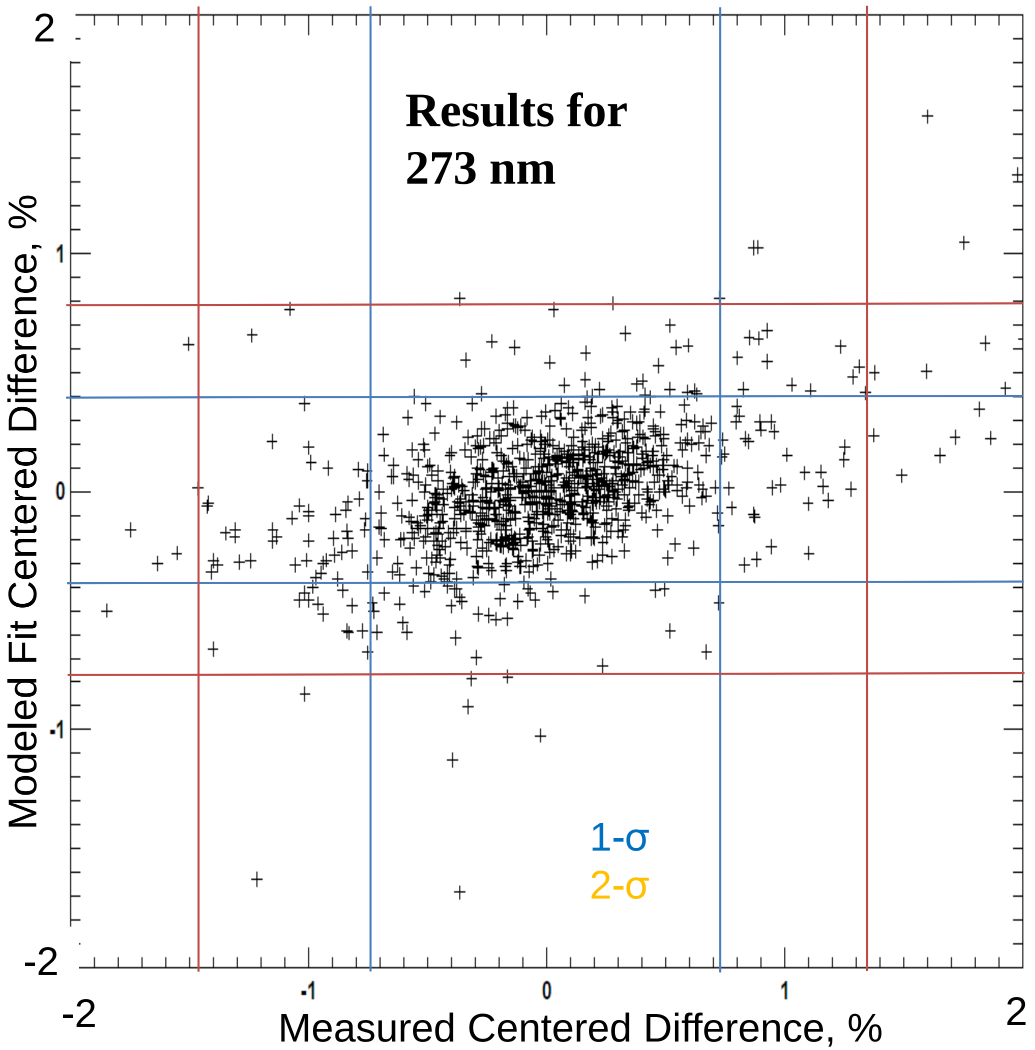
The filter process used an initial difference from a median test of the albedos followed by an iterative removal of terms using the absolute radiance differences from the fit.

The IDL code to calculate the fits is in the note pages.



Number and location (for scans with more two or more replaced outliers) of outliers for two days of S-NPP OMPS NP SDR data. Twelve wavelength intervals around 273 nm were used. The radiance/irradiance ratios for each spectral interval were fit with linear regression using a quadratic model in wavelength.

The filter process used an initial difference from a median test of the albedos followed by and iterative removal of data values using the absolute radiance difference from the fit.



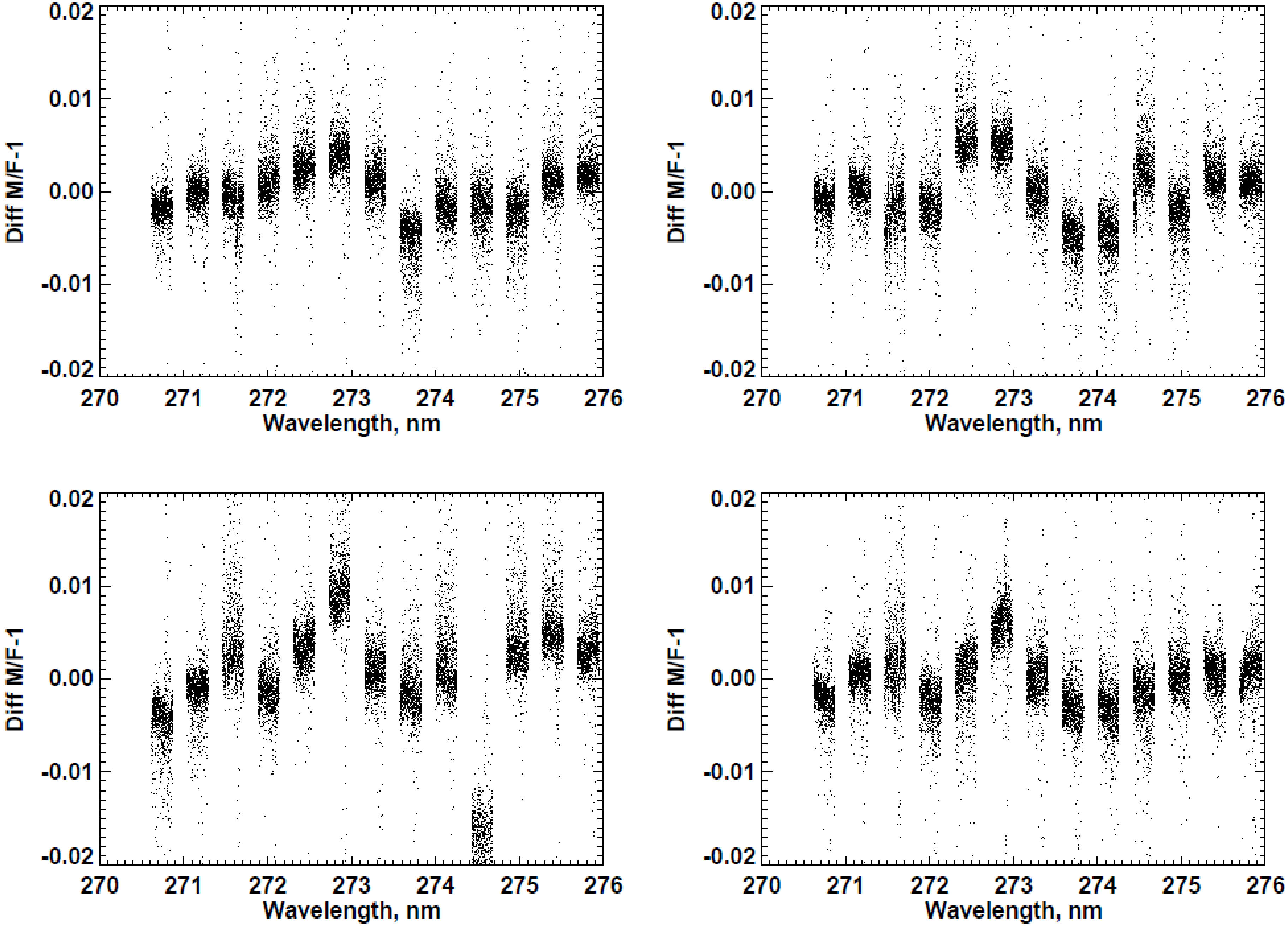
Nearest Neighbor Centered Differences

The along-track values at the V8Pro wavelengths for the middle (3rd) scan of five in a granule were compared to the averages of the 2nd and 4th ones. The plot to the left compares the percent differences for the measured results to the those for the model fits for the 273 nm channel.

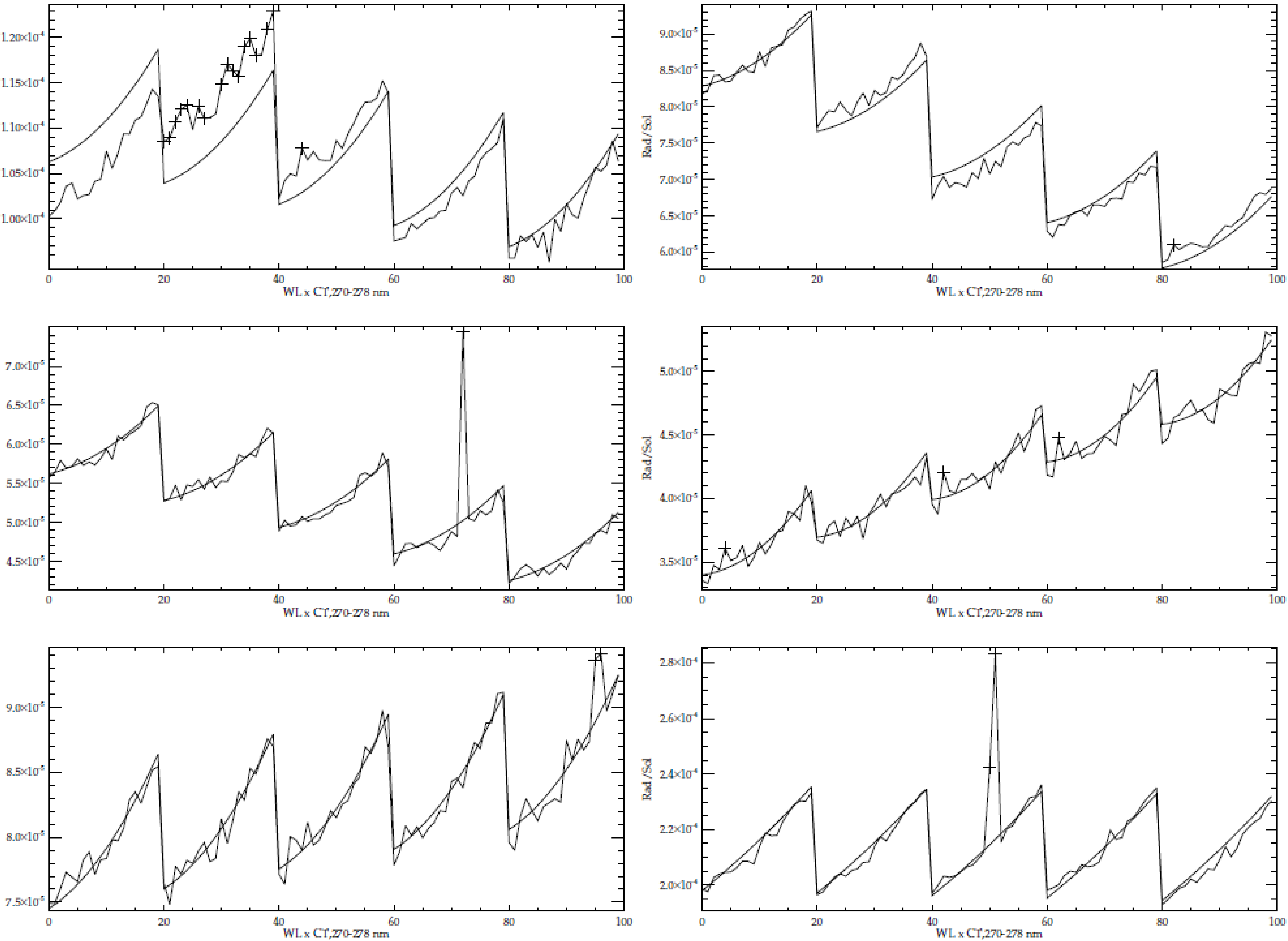
RMS Differences

nm	ModFit	Measured
253	1.04%	1.73%
273	0.39%	0.73%
283	0.32%	0.47%
288	0.26%	0.46%
292	0.14%	0.27%

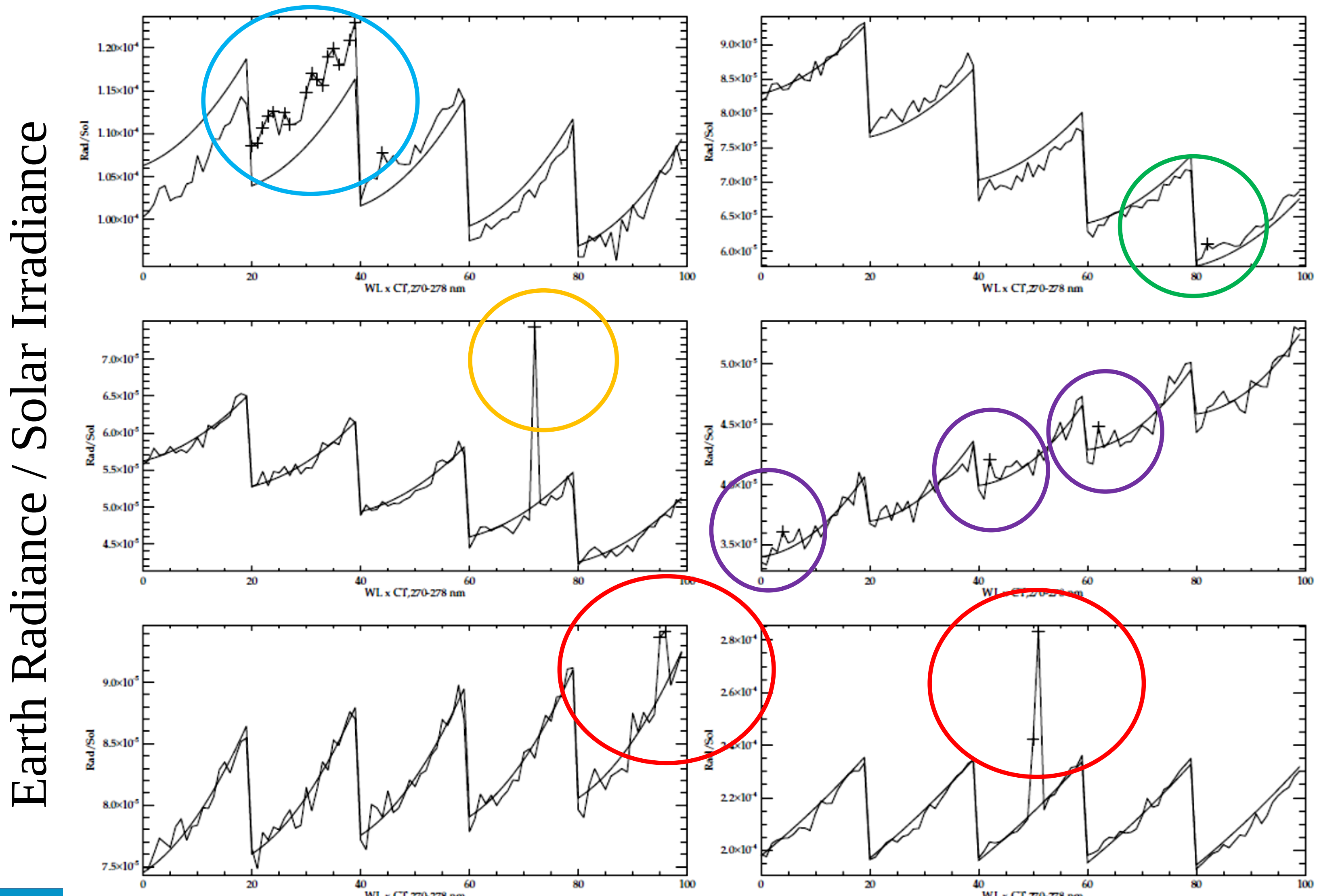
The model results show reduced noise for this statistic.



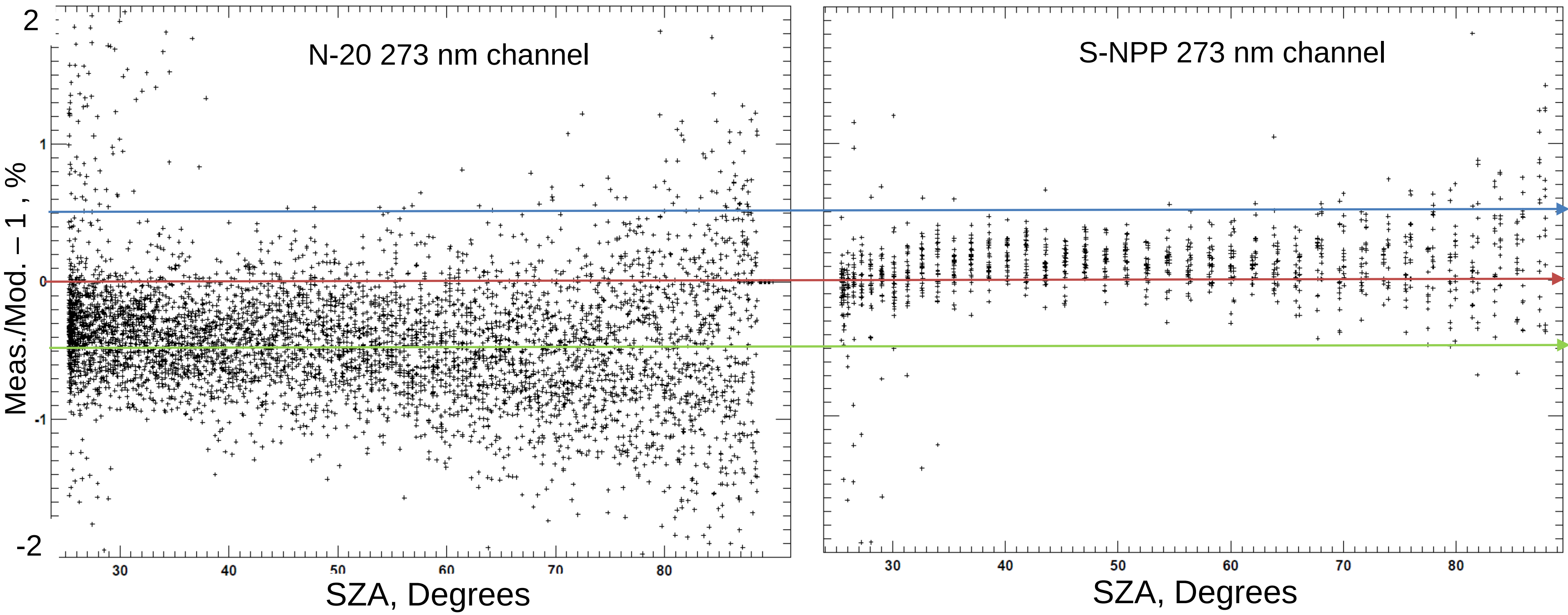
Diff M/F-1
0.02
0.01
0.00
-0.01
-0.02
270
271
272
273
274
275
276
Wavelength, nm
Diff M/F-1
0.02
0.01
0.00
-0.01
-0.02
270
271
272
273
274
275
276
Wavelength, nm
Diff M/F-1
0.02
0.01
0.00
-0.01
-0.02
270
271
272
273
274
275
276
Wavelength, nm
Diff M/F-1
0.02
0.01
0.00
-0.01
-0.02
270
271
272
273
274
275
276
Wavelength, nm


1.20×10⁻⁴
1.15×10⁻⁴
1.10×10⁻⁴
1.05×10⁻⁴
1.00×10⁻⁴
0 20 40 60 80 100
WL x CT,270-278 nm
Rad/Sol
9.0×10⁻⁵
8.5×10⁻⁵
8.0×10⁻⁵
7.5×10⁻⁵
7.0×10⁻⁵
6.5×10⁻⁵
6.0×10⁻⁵
0 20 40 60 80 100
WL x CT,270-278 nm
7.0×10⁻⁵
6.5×10⁻⁵
6.0×10⁻⁵
5.5×10⁻⁵
5.0×10⁻⁵
4.5×10⁻⁵
0 20 40 60 80 100
WL x CT,270-278 nm
Rad/Sol
5.0×10⁻⁵
4.5×10⁻⁵
4.0×10⁻⁵
3.5×10⁻⁵
0 20 40 60 80 100
WL x CT,270-278 nm
9.0×10⁻⁵
8.5×10⁻⁵
8.0×10⁻⁵
7.5×10⁻⁵
0 20 40 60 80 100
WL x CT,270-278 nm
Rad/Sol
2.8×10⁻⁴
2.6×10⁻⁴
2.4×10⁻⁴
2.2×10⁻⁴
2.0×10⁻⁴
0 20 40 60 80 100
WL x CT,270-278 nm

2-D Filter for 274 nm



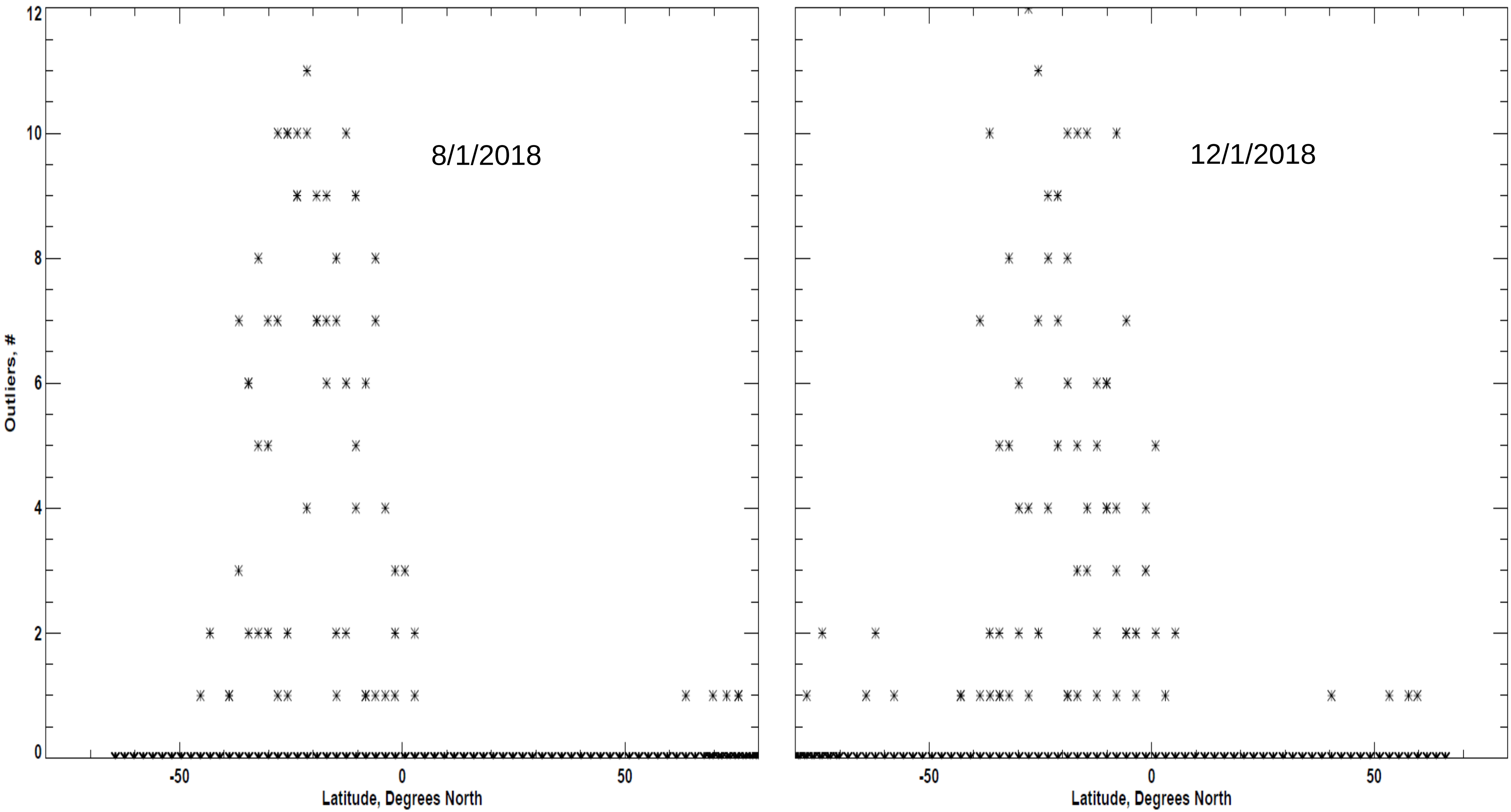
Measured minus Model “Bias” with SZA



Comparison of measured and modelled values for 273 nm channel for December 1, 2018. The figure on the left is NOAA-20 OMPS NP and the figure on the right is S-NPP OMPS NP.

F&IC Summary & Conclusions

- A simple model can be used to identify outliers from charged particle events.
- The single channel albedo values used in the V8Pro can be replaced by values from a fit over a local wavelength interval.
- This method will work well for small numbers of outliers.
- It will provide reduced noise estimates of the values even if no outliers are present.
- The method can also identify the presence of PMCs for the medium resolution NOAA-20 OMPS NP SDRs. Studies could be conducted comparing the aggregated FOVs to the individual ones to estimate the contamination of S-NPP OMPS NP SDRs and EDRs from PMC signals to add to the findings in [2] Thomas et al. 1991 and [3] Bak et al. 2016.


8/1/2018
12/1/2018
Outliers, #
Latitude, Degrees North
Latitude, Degrees North
12
10
8
6
4
2
0
-50
0
50

```
; Function to calculate fits for rad/irrad ratios for individual
; scans with up to five cross-track positions.
function radscanfit,sol,radg,wav,nwv,nct,del1,del2,wx,ay
; Put in a quadratic model with wavelength & linear with cross track.
;  nwv Number of wavelengths
;  nct Number of cross track
;  sol(nwv,nct) Solar irradiance
;  radg(nwv,nct) Earth radiance
;  wav(nwv,nct) wavelengths in nm
;  del1 radiance based limits on fit outlier sizes
;  del2 (1+del2) is relative outlier size compared to median albedo
;  wx is the wavelength of a retrieval channel
;  ay is the albedo value for the fit for that channel.
; SAMPLE INPUT for NOAA-20 OMPS NP
;  radg=fltarr(12,5)+datasdrpmc(100).radianceearth(4:15,0:4,2)
;  sol=fltarr(12,5)+datasdrpmc(100).solarflux(4:15,0:4)
;  wav=fltarr(12,5)+datasdrpmc(100).wavelengths(4:15,0:4)
;  del1=0.001 & del2=0.01 & nwv=12 & nct=5
;  wx=253.0 & ay=0.0
; Call
; radfit=radscanfit(sol,radg,wav,nwv,nct,del1,del2,wx,ay)
;  radfit is the same size and form as radg.
alb=radg*0.0
for k=0,nct-1 do alb(*,k)=radg(*,k)/sol(*,k)
;plot, alb,psym=3
     ; Median filter first
ma=median(alb)
;plot, alb/ma-1,psym=-3
ca=1.0+del2
wu=where(alb gt ma*ca,nwu)
if nwu gt 0 then alb(wu)=ma*ca
wd=where(alb lt ma/ca,nwd)
if nwd gt 0 then alb(wd)=ma/ca
; if nwu ge 5 or nwd gt 3 then print, nwu,nwd & oplot,alb/ma-1,psym=1
     ; Set up albedo values
yy=fltarr(nwv*nct)+reform(alb)
wz=dindgen(nwv*nct)+1.0
     ; Put in quadratic in wavelength
medwav=median(wav)
z1=wav-medwav
z2=z1^2
     ; Put in linear models with across track.
z3=dindgen(nct)/2.-1
if nct eq 1 then begin
  zz=dblarr(2,nwv)
  for i=0,nct-1 do zz(0,*)=z1(*,i)
  for i=0,nct-1 do zz(1,*)=z2(*,i)
endif
if nct gt 1 then begin
  zzt=dblarr(3,nwv,nct)
  for i=0,nct-1 do zzt(0,*,i)=z1(*,i)
  for i=0,nct-1 do zzt(1,*,i)=z2(*,i)
  for i=0,nwv-1 do zzt(2,i,*)=z3(0:nct-1)
  zz=dblarr(3,nwv*nct)+zzt
endif
rz=regress(zz,yy,wz,yyfit,const,sigma,ftest,relative_weight=1)
; LAPACK for FORTRAN Implementation
; http://www.netlib.org/lapack/explore-html/d8/dde/dgels_8f.html
; dgels (TRANS, M, N, NRHS, A, LDA, B, LDB, WORK, LWORK, INFO)
; TRANS='N' & M=nwv*nct & if nct eq 1 then N=3 & if NCT gt 1 then N=4 &
NRHS=1
; tzz=transpose(zz) & A=dblarr(M,N) & A(*,1:N-1)=tzz(*,0:N-2) &
; I can't tell if we need a constant term or not. I think we do.
; A(*,0)=1.0 & LDA=M
; B=YY (on input) &  rz=B(1:N-1) & const=B(0) (on output) & LDB=M
; WORK=dblarr(2*N+1) & LWORK=2*N+1  (I'm not sure about these.)
; INFO Integer output (0 Success, <0 illegal value, <0 No solution)
; if INFO eq 0 then yyfit=A#B
;
;plot, yy/yyfit-1
     ; Iterate after applying filter in radiance space.
yyt=yy
     ; For the first iteration, only remove positive outliers.
w=where(sol*(yy-yyfit) gt del1,nw)
if nw gt 0 then yyt(w)=yyfit(w)
rz=regress(zz,yyt,wz,yytfit,const,sigma,ftest,relative_weight=1)
yyt=yy
     ; For the second iteration, remove both positive and negative outliers.
w=where(abs(sol*(yy-yytfit)) gt del1,nw)
if nw gt 0 then yyt(w)=yytfit(w)
rz=regress(zz,yyt,wz,yytfit,const,sigma,ftest,relative_weight=1)

radfit=0.0*radg+yytfit
for k=0,nct-1 do radfit(*,k)=radfit(*,k)*sol(*,k)
     ; Find the Cross-track average fit value at the selected wavelength.
zx=wx-medwav
ay=0.0
ay=rz(0)*zx+rz(1)*zx*zx+const
     ; Note the cross track term's contribution to averages to 0.
;plot, radg/radgfit-1
     ; Should we set a flag if too many outliers are present?
;if nw gt 15 then stop
return,radfit
End
```

WHAT I KNOW (AND DON'T KNOW*) ABOUT WAVELENGTH SCALES, BANDPASSES AND DICHROICS

STUDY USING S-NPP OMPS AND NOAA-20 OMPS

L. Flynn, NOAA

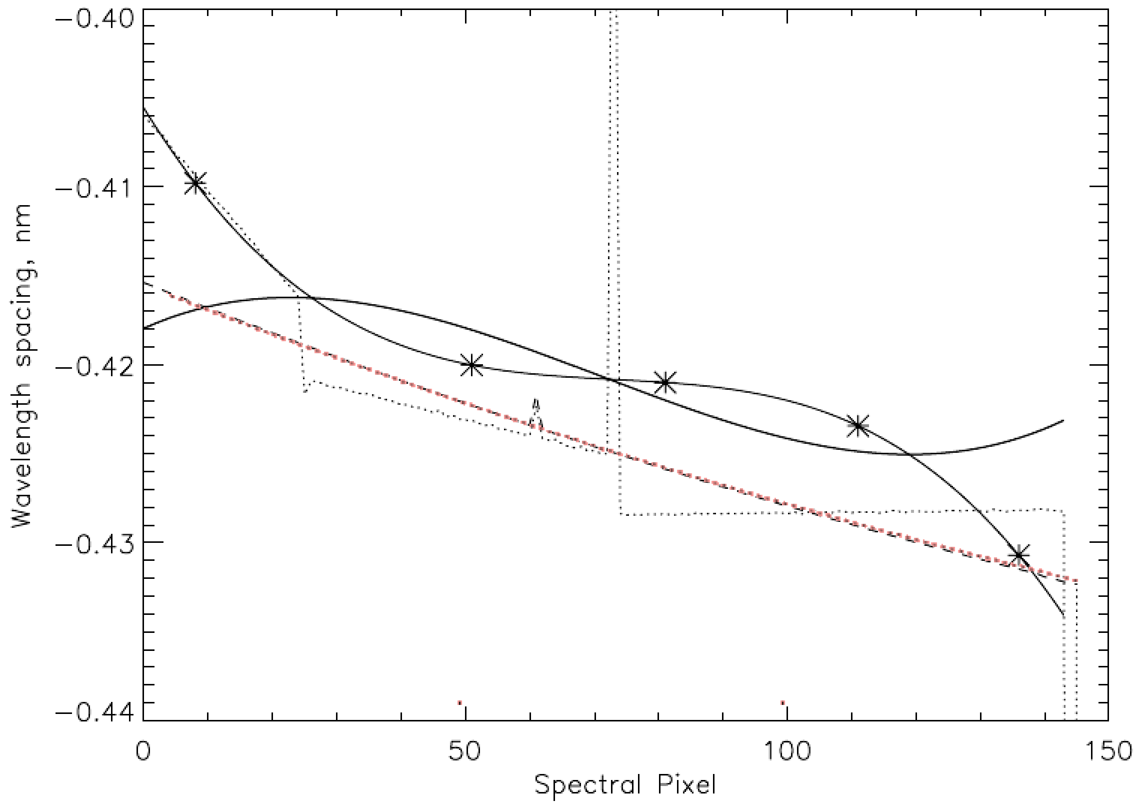
* Not an exhaustive list.

Wavelength Scales (Pixel Centers)

- The response of the instrument to a monochromatic input (e.g., Tunable Laser) at a range of spectral wavelengths, λ_m, and spatial locations, row j, is obtained.
- For each spatial row (or perhaps collection of adjacent spatial rows) above a threshold signal, the corrected (Dark, Offset and Pixel Response) counts are used to find the weighted-average spectral pixel, p_m, for each input wavelength, λ_m. Notice that this does not take into account any wavelength dependent throughput variations as each monochromatic data set is normalized relative to its total corrected counts.
- This gives a two dimensional data set of the form,

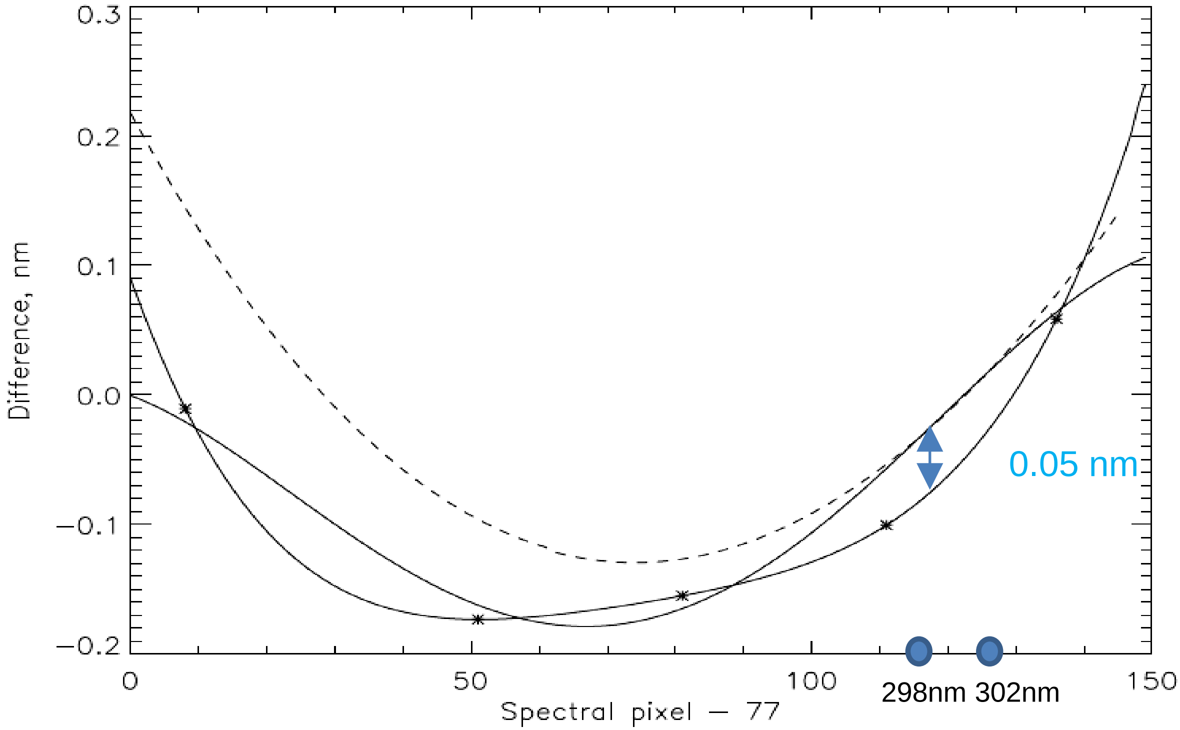
  $\{(\lambda_m,p_m)_j\}$

  for input wavelength λ_m and spatial row j.
- Inverting this, by considering wavelength as a function of pixel instead of pixel as a function of wavelength, and fitting with a two-dimensional model provides a way to assign wavelengths to pixels over the full active region. These are used to produce the Band Center data sets.
- The figures on the following slide compare the wavelength scales for OMPS NP for S-NPP and JPSS-1 (NOAA-20) to a simple linear model by examining their spacing. That is, the plots show the differences in the band centers of adjacent pixels (or macropixels). for spatial rows. If the wavelength scales were linear, these curves would be constants. The figure on the slide after the next one shows the differences of the wavelength scales with linear ones.



The S-NPP steps (dashed) are close to linear meaning that the wavelength scale is quadratic while the NOAA-20 steps (solid) follow a cubic meaning that its wavelength scale is quartic. The solid line without symbols are the NOAA-20 CBC data. The solid line with symbols are the NOAA-20 CBC data adjusted by the bandpass-weighted average wavelengths. The symbols in the figure show the locations of the five NOAA-20 spectral measurement sets. The red line is the S-NPP data adjusted by its bandpass-weighted average offsets.

Wavelength Scale versus Linear



The S-NPP (dashed) show the close to quadratic wavelength scale. The NOAA-20 (solid) follow a quartic wavelength scale. The solid line without symbols are the NOAA-20 CBC data. **The solid line with symbols (*) are the NOAA-20 CBC data adjusted by the bandpass-weighted average wavelengths**. The symbols in the figure show the locations of the five NOAA-20 spectral measurement sets.

Wavelength Scale Notes

- The CBC data set from the monochromatic laser analysis is good in that it should provide an accurate estimate of the wavelength that would have a weighted average response at a selected pixel's center.
- The analysis* method is insensitive to throughput variations with wavelength. For example, the results would be the same with or without a dichroic in the system in terms of throughput – the dichroic might also act as a broadening or scattering optical component which would be captured.
- The CBC data does not give the wavelength that would represent a pixel's weighted-average response wavelength (its bandpass-weighted wavelength centroid).

* This assumes that the analysis works with corrected counts (or counts converted to radiance by using the instrument's throughput for the input wavelength, not by using each pixel's average calibration coefficient).

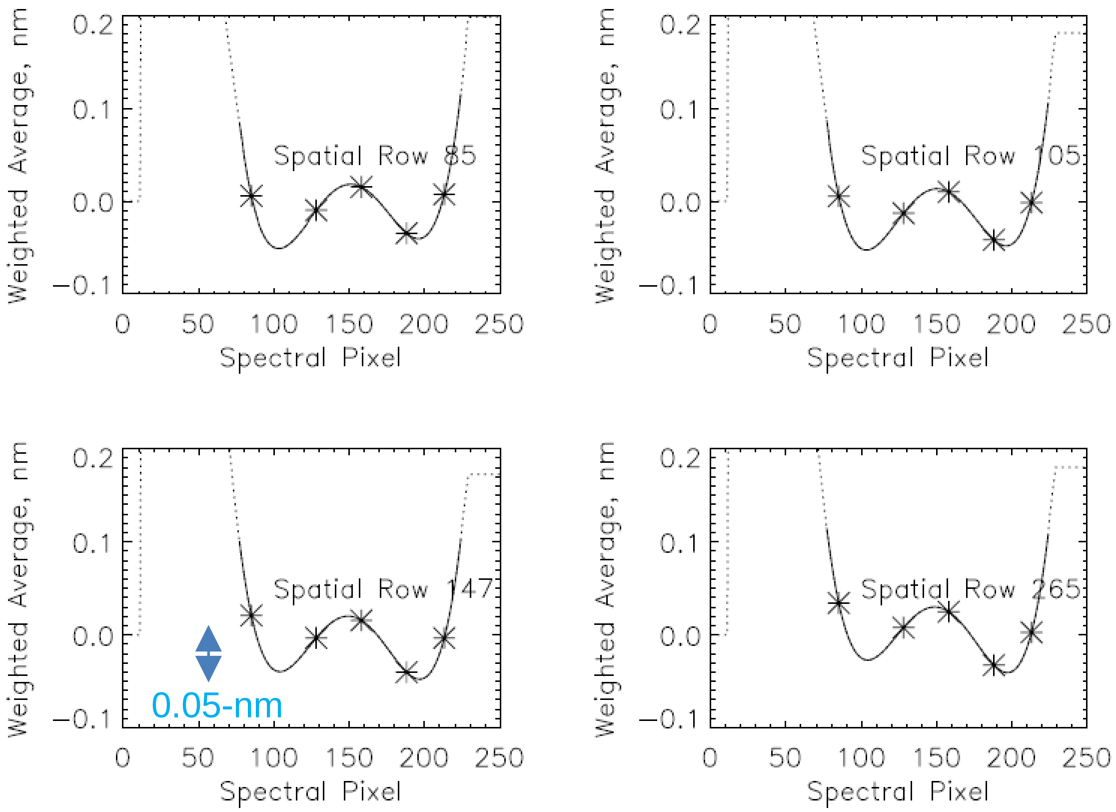
Bandpass offsets

- The bandpass-weighted average wavelength offsets in nm are computed as

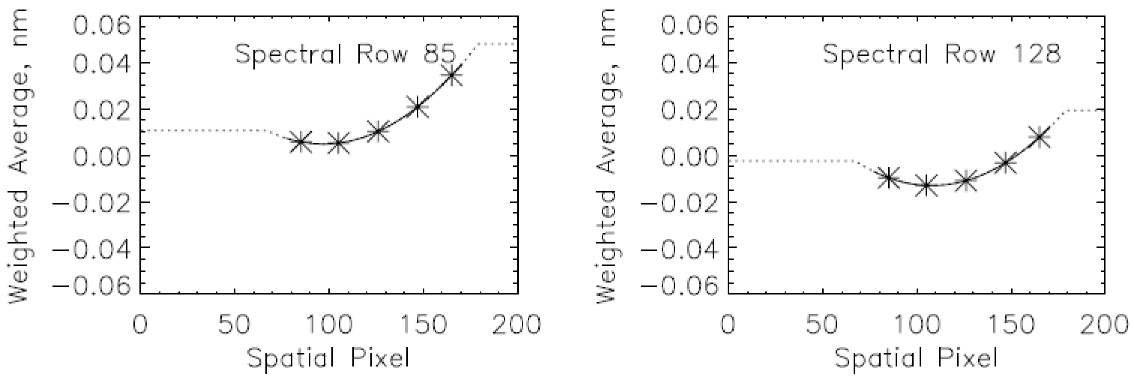
  $$sum\{BP_k*w_k\}/sum\{BP_k\}$$

  with w_k = (i-25)*0.1 and the sums taken over k=0 to 50, where BP is a set of 51 bandpass response values given every 0.1 nm centered at the pixel band centers from the earlier computations. Slices though the 2-D bandpass offset surface for NOAA-20 NP are displayed on the next two slides.
- The offsets for S-NPP are very small as evidenced by close agreement of the red and black dashed lines in Slide #3. That is the S-NPP bandpasses are centered in agreement with the wavelength scale.

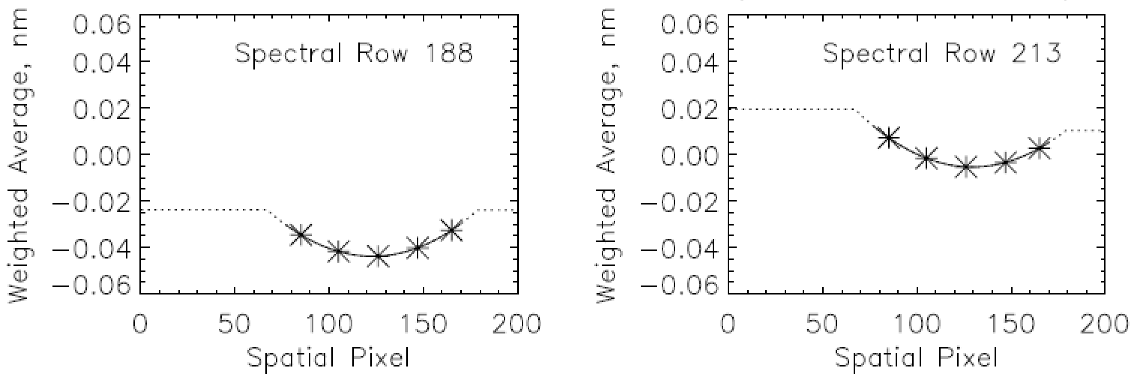
Weighted Average Bandpass Offsets for NOAA-20 Versus Wavelength Pixel



Weighted-Average Bandpass Offsets for NOAA-20 Versus Cross-track Spatial Pixel

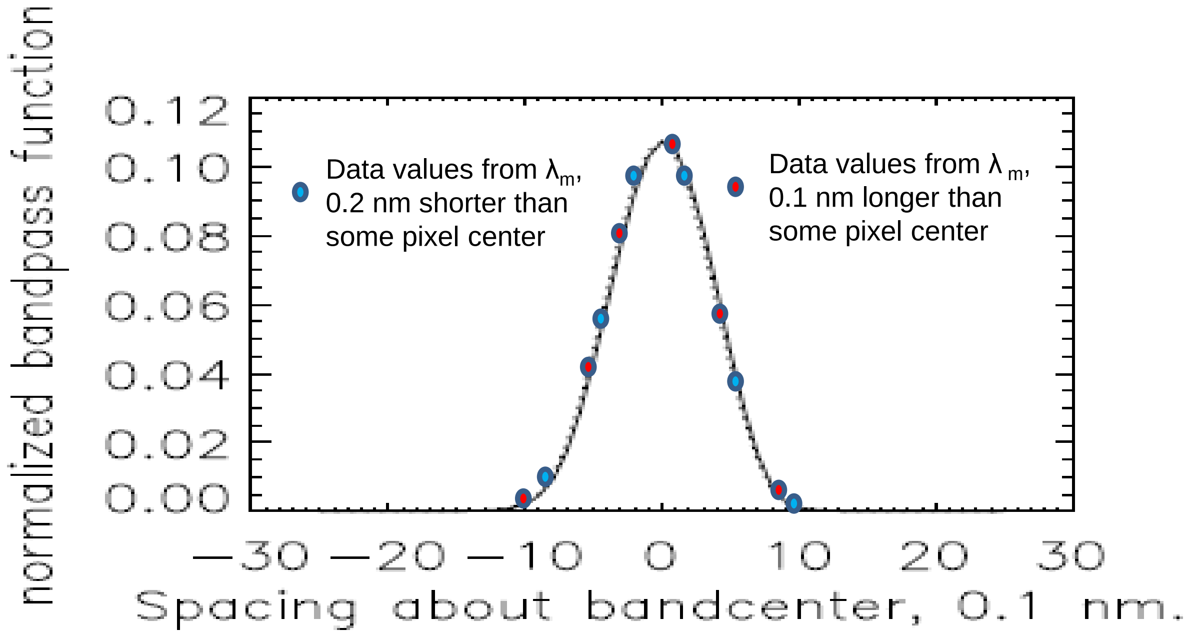


Solid lines denote the active region of the CCD array.



Bandpass Estimation (1)

- The same data used to get the wavelength scales can be used to get the non-wavelength-throughput-dependent bandpasses. One takes the measurements for a given laser wavelength input and again normalizes the total counts over some localized spectral and spatial region. The result is used to provide data points by using the laser input wavelength relative to the pixel centers computed earlier.



Bandpass Estimation (2)

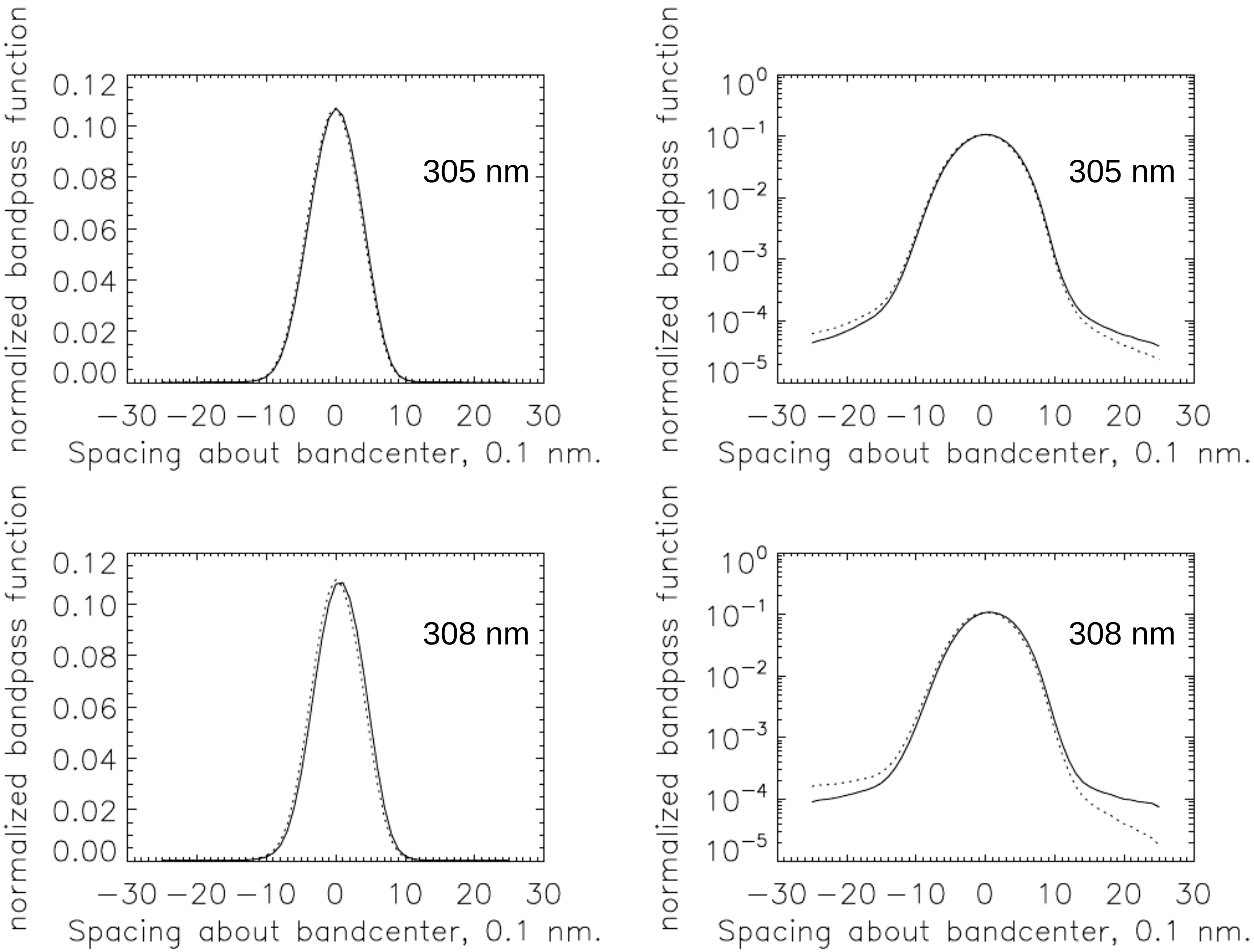
- There are two implicit key assumptions in this approach:

1. That the bandpasses change slowly in both spectral and spatial dimension so one can work with measurements over 12 spectral pixels and 8 spatial pixels.
2. That the normalization of a bandpass as sampled every 0.42 nm provides comparable values as the sampling is shifted relative to the center. (For the JPSS bandpasses, I have checked this by comparing the sums of every fourth bandpass value and it holds at the 0.2% level.)

- There is the further assumption that the corrected count responses for different pixels are consistent for a given specific photon energy / wavelength over the local analysis region.

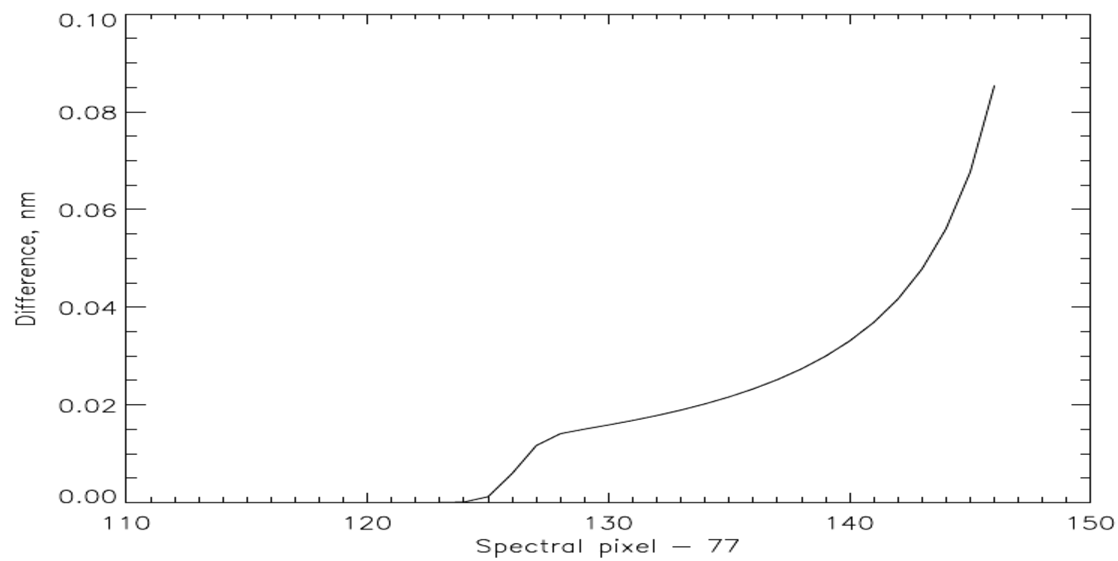
Bandpass Estimation (3)

- Again, these bandpasses will be the idealized instrument response functions without taking into account the wavelength-dependent throughput. One can adjust the bandpasses by using the relative wavelength dependent throughput to create the expected instruments bandpasses but this requires some assumptions about how the pixel count to radiance data are constructed from measurements.
- The pixel-dependent calibration constants were used as a proxy for wavelength-dependent throughput variations to see how much the real bandpasses would be changed. The pixel level constants were used by assigning the conversion value to the central wavelength. These were linearly interpolated to create a set of values with 0.1-nm spacing about the central wavelength of a pixel. The full set of values are convolved with the current bandpass data for that pixel and central wavelength to produce throughput-weighted bandpass values.
- The figures on the next page compare unadjusted (Solid) and adjusted (Dotted) bandpasses with linear (Left) and log (Right) scales for 305 nm (Top) and 308 nm (Bottom) for S-NPP OMPS NP.


normalized bandpass function
0.12
0.10
0.08
0.06
0.04
0.02
0.00
305 nm
−30 −20 −10 0 10 20 30
Spacing about bandcenter, 0.1 nm.
normalized bandpass function
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
305 nm
−30 −20 −10 0 10 20 30
Spacing about bandcenter, 0.1 nm.
normalized bandpass function
0.12
0.10
0.08
0.06
0.04
0.02
0.00
308 nm
−30 −20 −10 0 10 20 30
Spacing about bandcenter, 0.1 nm.
normalized bandpass function
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
308 nm
−30 −20 −10 0 10 20 30
Spacing about bandcenter, 0.1 nm.

Bandpass Offsets from the Dichroic

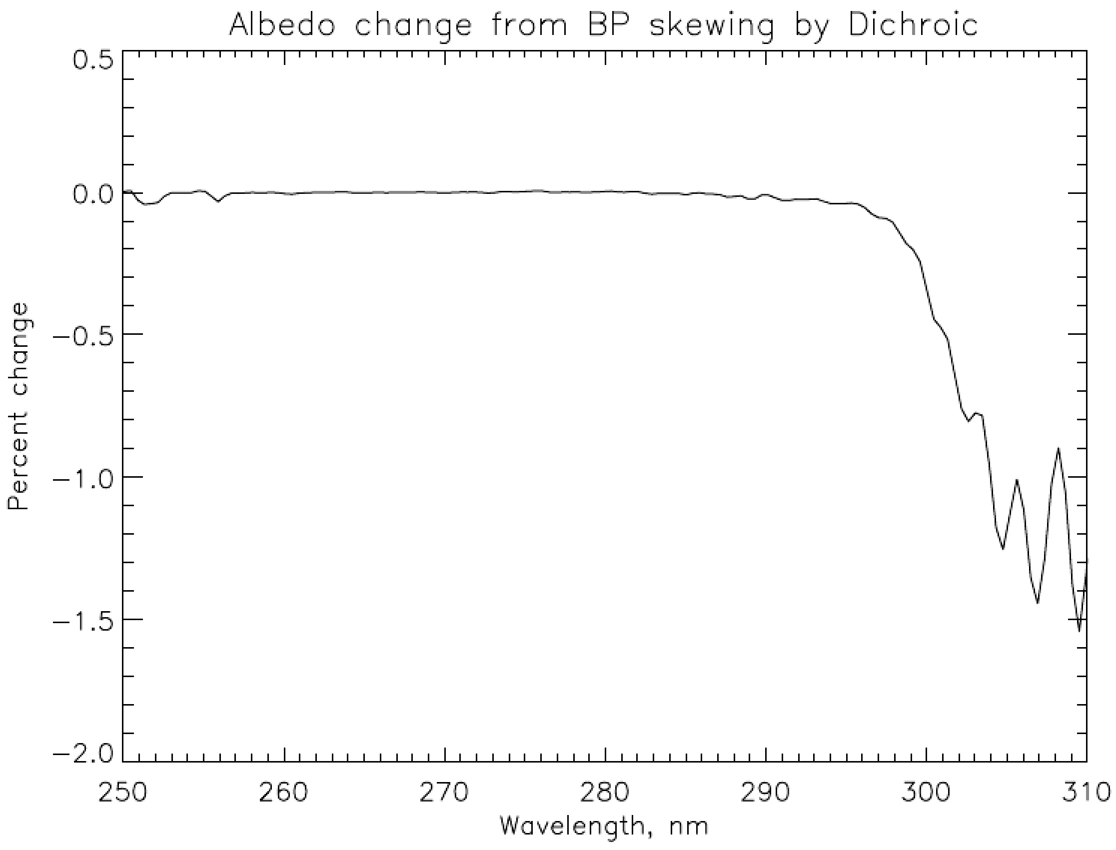
- The throughput adjustments creates bandpasses with different centering – different weighted-average bandpass wavelength offsets. The figure below shows the differences in the weighted-average bandpass centers, old – new, for S-NPP OMPS NP.



293 nm 310 nm

Applying the new Bandpasses

- Since the albedo is rapidly changing over the 300 nm to 310 nm interval, changing the bandpasses will affect the Solar and Earth View data differently leading to changes in the expected albedo. That is, there will be significant differences in an RT instrument table created by the two sets of bandpasses.
- The figure on the next slides uses a single set of measured NP radiance and irradiance spectra interpolated to higher density and convolved with the old and new bandpasses to estimate the albedo changes.
- The sign of these changes will switch from the NP to the NM over the 300 nm to 310 nm interval, as the throughput gradients from the dichroic are in the opposite directions.

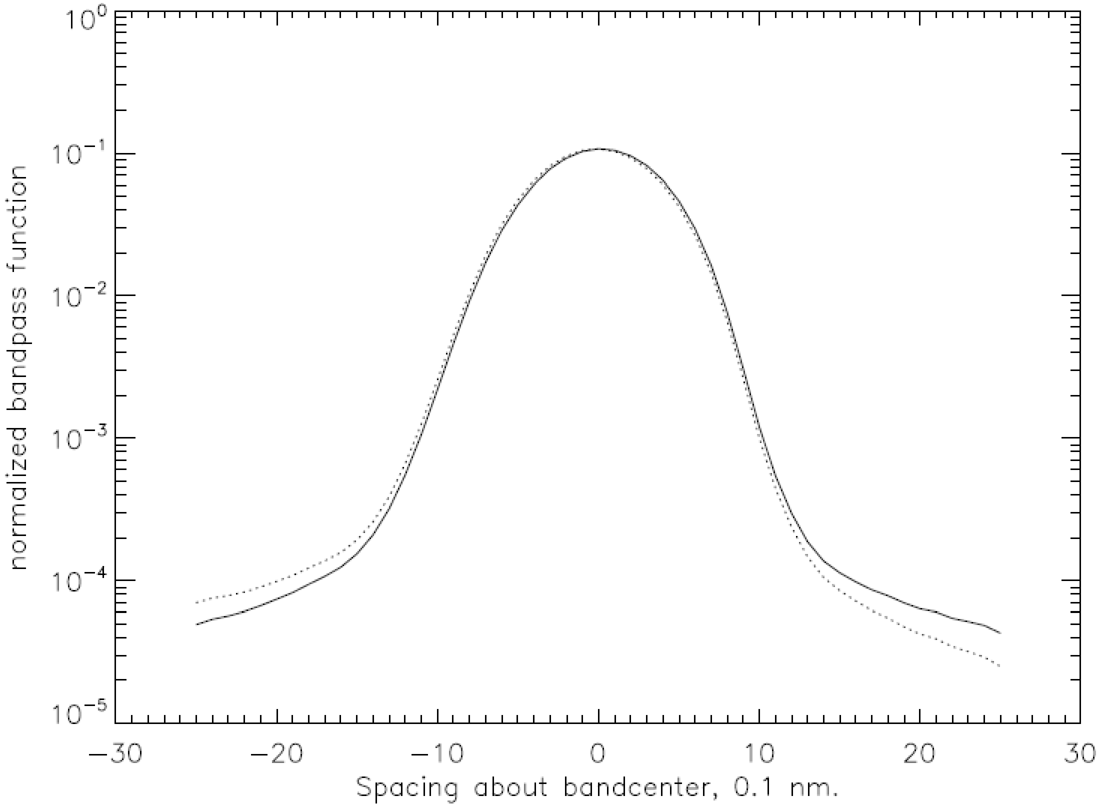

Albedo change from BP skewing by Dichroic
0.5
0.0
−0.5
−1.0
−1.5
−2.0
Percent change
250
260
270
280
290
300
310
Wavelength, nm

Open Questions

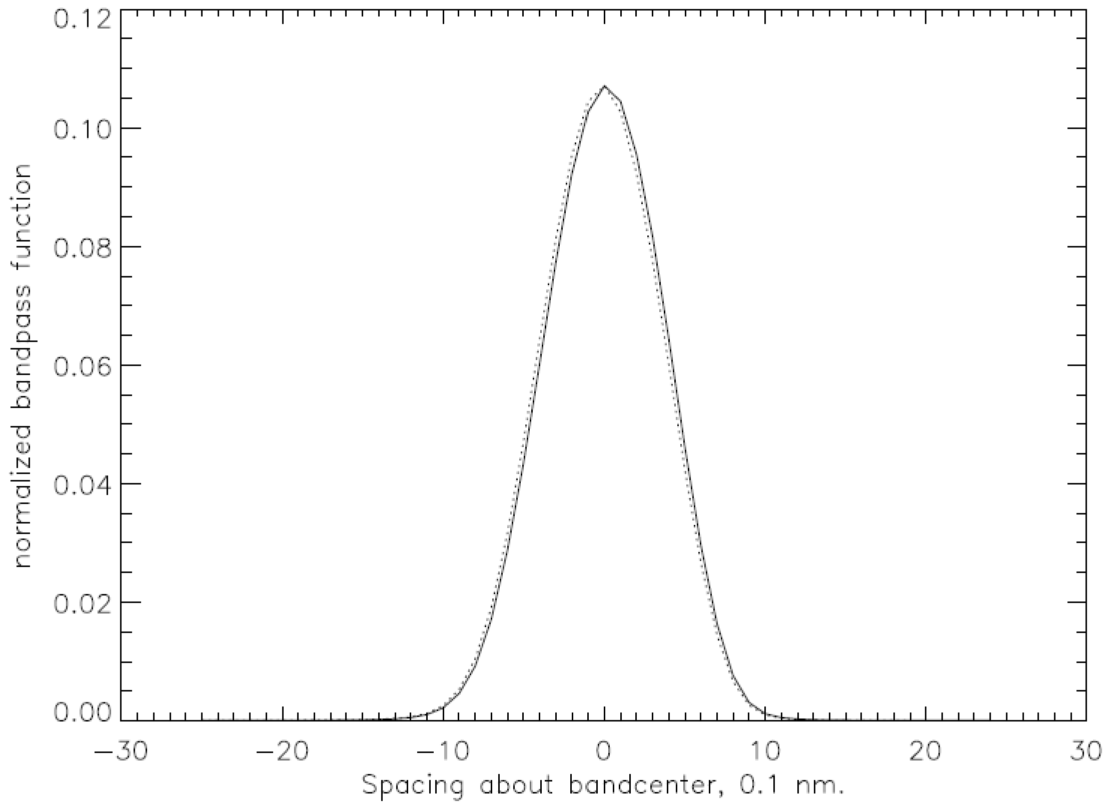
- Why does the S-NPP data show a good fit by a quadratic in wavelength and the bandpasses have small offsets*? Or, Why do the NOAA-20 data need a quartic to get a good fit and the bandpasses have large offsets^?
- Why don't the provided bandpasses show the dichroic skewing? Will the throughput adjustments by using skewed bandpasses improve the RT forward model albedo comparisons and OMPS NM/NP agreement in the overlap region for S-NPP?
- How accurately can we estimate the wavelength scales in-orbit?

* I still need to check the S-NPP data to see how well the observed values are fit by the provided characterizations.

^ I expect/assume that the bandpasses should be consistent with the bandcenters from the analysis of the same set of laser measurements.



normalized bandpass function
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
−30
−20
−10
0
10
20
30
Spacing about bandcenter, 0.1 nm.


0.12
0.10
0.08
0.06
0.04
0.02
0.00
normalized bandpass function
−30
−20
−10
0
10
20
30
Spacing about bandcenter, 0.1 nm.